Open access • Journal Article • DOI:10.1007/BF00375026

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Published on: 01 Sep 1992 - Archive for Rational Mechanics and Analysis (ARCHIVE FOR RATIONAL MECHANICS AND ANALYSIS)

Topics: Diffusionless transformation, Bainite, Martensite, Austenite and Microstructure

SELF-ACCOMMODATION IN MARTENSITE

By

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IMA Preprint Series # 879

October 1991

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ABSTRACT

The shape-memory effect is a phenomenon wherein an apparently plastically deformed specimen recovers all strain when heated to above a critical temperature. This is observed in some crystalline solids that undergo the martensitic phase transformation. The martensitic transformation is a temperature induced, diffusionless solid to solid phase transformation involving a change in crystalline symmetry. Shape-memory materials are able to transform from the high temperature austenite to the low temperature martensite phase without any apparent change in shape. This is known as self-accommodation. Though there is a change of shape at the microscopic level, the martensitic variants arrange themselves in such a microstructure that there is no macroscopic change in shape. Apart from being an inherent part of the one-way shape-memory effect, it can be argued that self-accommodation is also important for the reversibility of transformation in polycrystals and for easy nucleation of martensite during cooling. Using a continuum theory based on finite thermoelasticity, we investigate which materials can form a self-accommodating microstructure. In particular, necessary and sufficient conditions that the lattice parameters of a material have to satisfy in order that it is able to form a self-accommodating microstructure are derived. The analysis here is significantly different from the previous studies because it makes no *a priori* assumption on the microstructure. The main result states that if the austenite is cubic, the material is self-accommodating if and only if the transformation is volume preserving. On the other hand, if the symmetry of the austenite is not cubic, it is not possible to construct any microstructure that is self-accommodating unless the transformation strain or the Bain strain satisfies additional, rather strict, conditions. These results show good agreement with the available experimental data. Necessary conditions are derived using the minors relations, while sufficiency is demonstrated by explicit construction.

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§1. INTRODUCTION

One-way shape-memory is the ability of a material to remember its shape above a critical temperature. This phenomenon is observed in certain crystalline solids, typically metallic alloys. Below the critical temperature, the alloy is extremely malleable - undergoing apparently plastic deformations with strains as large as 10% under very small forces. It is therefore possible to deform a piece of shape-memory material into a variety of new shapes. However, all the strain is recovered when it is heated to above the critical temperature. Cooling from above to below the critical temperature does not cause any macroscopic shape change and the cycle can be repeated. This is shown schematically in Figure 1.1.

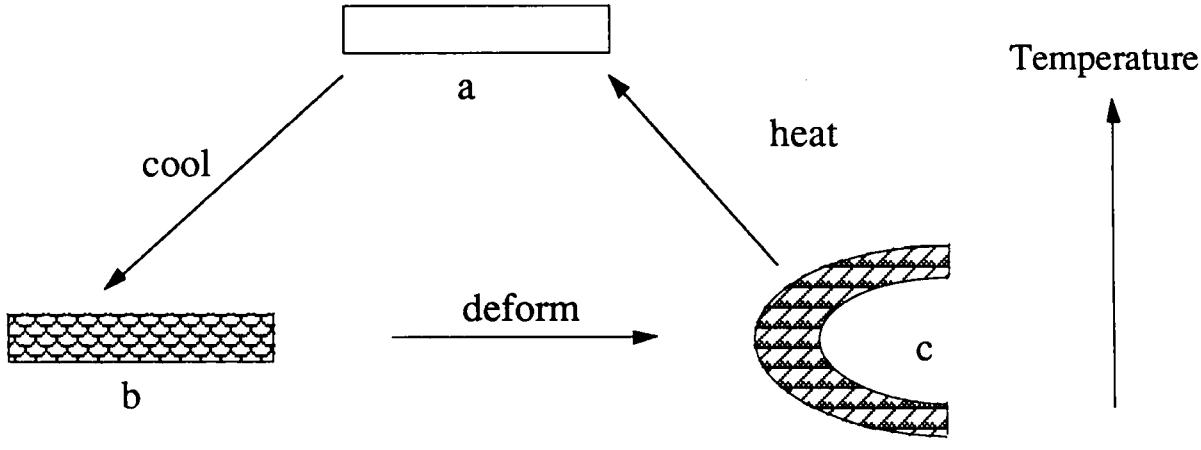

Figure 1.1: The shape-memory effect.

Intensive experimental and crystallographic investigation during the 1960s and the 70s revealed that the heart of the effect lies in the reversible or "thermoelastic" martensitic transformation that these crystalline solids undergo. A martensitic transformation is a temperature induced first order diffusionless phase transformation between the high temperature austenite phase and the low temperature martensite phase. The critical temperature of the shape-memory effect is the transformation temperature. In these solids, the lattice of the austenite has higher symmetry than that of the martensite. This gives rise to more than one variant of martensite. Variants are identical crystal lattices which are oriented differently with respect to the austenite. The variants

may arrange themselves in fine microstructure in order to satisfy imposed boundary conditions. These microstructures are coherent and free of internal stresses on a macroscopic scale.

Consider a specimen of a given shape in Figure 1.1a. It is in the austenite phase. On cooling, the austenite transforms to the martensite. However, the variants of martensite arrange themselves in such a manner that there is no macroscopic change in shape (Figure 1.1b). When loads are applied to the martensite, it deforms by converting one variant to another and forming new microstructures (Figure 1.1c). On heating, each variant transforms back into the austenite. Since there is only one variant of austenite, all the strain is recovered and the specimen goes back to its original shape (Figure 1.1a).

As mentioned above, the variants of martensite in a shape-memory material arrange themselves in such a microstructure that there is no macroscopic change in shape during the transformation from austenite to the martensite. Therefore, though there is a deformation at the microstructural scale due to the transformation, the variants "accommodate each others strains" so that there is no change in shape at the macroscopic level. This is known as *self-accommodation.* A *self-accommodating microstructure* is a coherent arrangement of martensitic variants occupying a region whose boundary suffers no displacement with respect to the austenite. Thus, it is possible to embed a self-accommodating microstructure in a sea of austenite in a coherent manner without introducing macroscopic stresses. A recent paper of Tan and Xu[63] contains striking optical micrographs of such islands of martensite surrounded by the austenite in an alloy of copper, aluminum and nickel (Cu - 14 wt. % Al - 4.2 wt. % Ni). A material that can form a self-accommodating microstructure is called a *self-accommodating material.* Wayman and others have emphasized the importance of self-accommodation to the shape-memory effect[58].

Apart from the fact that self-accommodation is an inherent part of the shape-memory phenomenon, it arguably plays a crucial role in making the transformation reversible or thermoelastic. The following argument is intuitively appealing. A typical piece of shape-memory material is a polycrystal consisting of a large number of randomly arranged grains. Owing to the random arrangement and shapes of the grains, it is easy to believe that any change in the shapes of the grains would cause some mismatch at the grain boundaries resulting in internal stresses and, possibly, cracks. The possible presence of temperature gradients further complicates the situation. Thus, a change in shape during transformation may be hostile towards reversibility. On the other hand, the property of self-accommodation is certainly sufficient to prevent any mismatch in a polycrystal. Similarly, it may also be argued that self-accommodation is important for the easy nucleation of the martensite during cooling. Any nucleus of martensite that forms in the interior of the specimen is completely surrounded by the austenite. Only self-accommodating materials can

do this in a coherent and stress-free manner. Thus, internal nucleation is likely only in self-accommodating materials.

Studying common shape-memory alloys using the crystallographic theory of martensite, Tas, Delaey and Deruyterre[65] and Saburi and Wayman[58] proposed certain microstructures as self-accommodating. The central idea in both their analysis is that of a "self-accommodating plate group". This is explained in the appendix. It turns out that these microstructures are either incoherent or require macroscopic internal stresses. Moreover, their analysis does not determine which materials can and which materials cannot form a self-accommodating microstructure. It is clear that not every material that undergoes martensitic transformation is self-accommodating. For example, consider a material where the volume of the martensite is smaller than that of the austenite. In this material, is not possible to embed any microstructure of martenisite in a sea of austenite in a coherent manner without introducing macroscopic stresses. Therefore, this material is clearly not self-accommodating. The central issue of this paper is to find necessary and sufficient conditions on the lattice parameters of a material in order that it be self-accommodating.

The main result is shown in Table 3.1. A surprising consequence of our results is that even though it is the variants of martensite that participate in the self-accommodating microstructure, the conditions for self-accommodation as stated in Table 3.1 depend only on the symmetry of the austenite. As explained above, volume preservation during transformation is necessary for self-accommodation. It turns out that volume preservation during transformation is also sufficient for self-accommodation if the symmetry of the austenite is cubic. In fact, in the case of cubic austenite, it is always possible to construct a microstructure which is a pure dilatation with respect to the austenite. The amount of dilatation, of course, depends on the transformation volume change. However, if the symmetry of the austenite is not cubic, the lattice parameters of the material have to satisfy additional restrictions which are extremely stringent and non-generic. For example, in a tetragonal to orthorhombic transformation, in addition to volume preserving transformation, it is necessary (and sufficient) that there is no stretch in the direction of the "c-axis" of the tetragonal lattice. In summary, materials with cubic austenite have to satisfy a rather easy constraint while materials with non-cubic austenite have to satisfy very restrictive conditions in order to be self-accommodating. This may be the reason why every shape-memory material that I have found in the literature has cubic austenite and undergoes very small volume change during transformation.

Following the work of Ericksen and James amongst others[9,10,12,19,22-29,37-39,56,57,71], these crystals are modelled as thermoelastic solids. This continuum model is derived by linking the movement of the atoms to the macroscopic deformation using the Cauchy-

Born hypothesis[27,71]. Different configurations of the crystal are regarded as deformations from a chosen reference configuration. Section 2 explains the constitutive assumptions and develops the mathematical concepts used in the analysis. The main constitutive assumption is that there is a free energy per unit reference volume which depends on the local change in shape measured by the deformation gradient and the temperature. At the transformation temperature, the energy has wells in the space of deformation gradients corresponding to both the austenite and the martensite phases. The position of the wells is determined by the lattice parameters of the crystal lattices of both phases. Because of the wells, the energy is not "quasiconvex" and it is possible that certain minimization problems with prescribed homogeneous boundary conditions have no solution. In such cases, it is necessary to study minimizing sequences. The minimizing sequences in which the gradients remain uniformly bounded are interpreted as coherent fine scale microstructure. The necessary and sufficient conditions for self-accommodation are derived in Section 3. The "minors relations", which are consequences of the weak continuity of the minors of the gradient are used to derive the necessary conditions. The sufficiency is demonstrated by constructing special microstructures involving multiple levels of laminates. Section 4 contains some comparison of theory and experiment. In Section 5 we discuss the implications of the results in Table 3.1 for the shape-memory phenomenon. It ends with a speculative discussion of why actual materials do not exhibit as many levels of laminates as required by the constructions in Section 3.

We use the minors relations in Section 3 to derive necessary conditions that turn out to be sufficient for the existence of a self-accommodating microstructure. The minors relations are a statement of certain special properties of the minors or subdeterminants of matrices. Any set of matrices that participate in a microstructure must satisfy the minors relations. Therefore, the minors relations are an easy way of deriving necessary conditions for the existence of certain microstructures. However, it is well-known that there are matrices which satisfy the minors relations but do not participate in any microstructure[6,31,59]. Therefore, in general the conditions derived using these relations are not sufficient to guarentee the existence of microstructure. However, they often turn out to be sufficient, as they do in our problem. Ball and James[10] and James and Kinderlehrer[39] amongst others have also used these relations to derive conditions that turn out to be sufficient in problems involving martensites. Ball[5,8] has used the weak continuity of the minors in problems of elasticity. Avellaneda, Charkaev, Lurie and Milton[4] amongst others have used the same properites of the minors to obtain optimal bounds on the effective properties of composites and polycrystals. Murat and Tartar[50-52,64] have used the weak continuity of the minors to develop what they call "compensated compactness". Thus, these minors relations appear to be extremely useful in problems involving microstructure.

Before we begin, a word about the notation and conventions which are used unless otherwise mentioned. Scalars are denoted using Greek letters. Bold faced Roman letters denote vectors, while bold faced Roman capitals denote tensors or matrices. $\mathbf{1}$ denotes the identity tensor. All vectors with hats, e.g. $\hat{\mathbf{i}}$ are unit vectors. The subscripts or indices i,j,k,l are integers from 1 to 3, while I,J,K,L are integers between 1 and some specified integer. The superscripts j and k are used to index sequences and run from 1 to infinity, while superscripts n,m and s denote some fixed positive interger. SO(3) is the group of all rotations ($\mathbf{Q}^T\mathbf{Q} = \mathbf{Q}\mathbf{Q}^T = \mathbf{1}$ and $\det \mathbf{Q} = +1$) in three dimensions. $\mathbf{R}[\theta,\mathbf{e}]$ denotes a counterclockwise rotation of $\theta°$ about $\mathbf{e}$.

§2. CONSTITUTIVE ASSUMPTIONS AND MICROSTRUCTURE

Consider a specimen consisting of undistorted austenite at the transformation temperature. Let it occupy an open, connected and bounded domain $\Omega \subset \mathbb{R}^3$ such that $\partial\Omega$ is Lipschitz. Choose this as the reference configuration. Since the phase transformation is structural and does not involve any diffusion or change in composition, all the configurations of the crystal can be described as the deformation $\mathbf{y} : \Omega \to \mathbb{R}^3$ of this reference configuration. For example, the transformation from austenite to martensite is described by the homogeneous deformation $\mathbf{y}(\mathbf{x}) = \mathbf{S}_1\mathbf{x}$. $\mathbf{S}_1$ is known as the transformation strain. It satisfies $\det \mathbf{S}_1 > 0$. For a given material, it depends on the lattice parameters of both the austenite and the martensite and may be determined experimentally.

Assume that there is a free energy per unit reference volume $\phi(\mathbf{F},\theta)$ which depends on the change of shape measured by the deformation gradient and the temperature. The total energy of the crystal $\mathcal{E}_\Omega[\mathbf{y},\theta]$ under the deformation $\mathbf{y}(\mathbf{x})$ at the temperature θ is given by

$$\mathcal{E}_\Omega[\mathbf{y},\theta] = \int_\Omega \phi(\nabla\mathbf{y}(\mathbf{x}),\theta)\, d\mathbf{x}.$$

Let $\phi(\mathbf{F},\theta)$ be defined on $\mathcal{D} \times \Theta^*$, where $\mathcal{D}$ is a suitable open, bounded subset of all second order tensors in three dimensions and $\Theta \subset \mathbb{R}$ is an open interval containing the transformation temperature θ_o. Also assume that for each $\theta \in \Theta$, the restricted function $\phi(\mathbf{F},\theta)$ is continuous on $\mathcal{D}$. Restricting the definition of ϕ to $\mathcal{D}$ instead of the space of all tensors is motivated by the molecular theory. According to that, it is necessary to restrict the domain of deformation gradients to some "Pitteri neighborhood" in order to obtain a finite material symmetry group[10,25,26,34,56,57]. We assume that $\mathcal{D}$ is bounded and that $\mathbf{1}$ and $\mathbf{S}_1$ belong to $\mathcal{D}$.

At a given temperature, the configuration observed in a crystal subjected to a displacement boundary condition $\mathbf{y}(\mathbf{x}) = \mathbf{y}_o(\mathbf{x})$ on $\partial\Omega$ is given by the deformation that minimizes $\mathcal{E}_\Omega[\mathbf{y},\theta]$ amongst all deformations $\mathbf{y} \in \mathcal{S}$ that satisfy $\mathbf{y}(\mathbf{x}) = \mathbf{y}_o(\mathbf{x})$ on $\partial\Omega$. $\mathcal{S}$ is a suitable class of functions. The answer to the above minimizing problem depends on the choice of $\mathcal{S}$. We are interested in coherent deformations that do not open up holes or cracks in the specimen. At the same time however, we would like to allow jumps in the gradient. Lipschitz functions, or equivalently, functions in $W^{1,\infty}(\Omega\,;\,\mathbb{R}^3)$ are the best suited to describe such deformations. Finally,

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* x denotes the cartesian product.

we do not want the material to collapse into a point. This is ensured by assuming that the deformation gradient has a positive determinant. All of the above motivate the following choice.

$$\mathcal{S} = \{ \mathbf{y} \in W^{1,\infty}(\Omega ; \mathbb{R}^3) \mid \nabla \mathbf{y}(\mathbf{x}) \in \mathcal{D} \} \qquad \text{where}$$

$W^{1,\infty}(\Omega ; \mathbb{R}^3)$ is the Sobolev space of mappings $\mathbf{y} : \Omega \to \mathbb{R}^3$ with finite norm

$$\| \mathbf{y} \|_{1,\infty} \stackrel{\text{def}}{=} \operatorname*{ess\,sup}_{\mathbf{x} \in \Omega} \{ |\mathbf{y}(\mathbf{x})| + |\nabla \mathbf{y}(\mathbf{x})| \}.$$

For future use, we make the following definition here. Let m be any positive integer. $L^\infty(\Omega ; \mathbb{R}^m)$ is the Banach space of mappings $\mathbf{F} : \Omega \to \mathbb{R}^m$ with finite norm

$$\| \mathbf{F} \|_\infty \stackrel{\text{def}}{=} \operatorname*{ess\,sup}_{\mathbf{x} \in \Omega} |\mathbf{F}(\mathbf{x})|.$$

We do not expect rigid body rotations of the crystal to change its energy. Similarly, the austenite lattice contains crystallographically indistinguishable directions. In order that our free energy reflects these, we make the following assumptions. Firstly, assume that $\mathcal{D}$ has the following invariance.

$$\mathbf{F} \in \mathcal{D} \qquad \Rightarrow \qquad \mathbf{QFR} \in \mathcal{D} \qquad \forall\, \mathbf{Q} \in SO(3) \quad \text{and} \quad \forall\, \mathbf{R} \in \mathcal{P}_a.$$

Here, $\mathcal{P}_a$ is the point group of the austenite lattice. The point group of a lattice is the group of rotations that map a lattice back into itself. Corresponding to the different crystal systems, there are seven point groups, all of which are finite. For example, the point group of the cubic lattice consists of the 24 rotations that map a cube back into itself. Now, assume that the free energy $\phi(\mathbf{F},\theta)$ has the following invariance.

Frame indifference: $\phi(\mathbf{F},\theta) = \phi(\mathbf{QF},\theta) \qquad \forall\, \mathbf{Q} \in SO(3), \qquad \forall\, \theta \in \Theta.$ (2.1)

Material Symmetry: $\phi(\mathbf{F},\theta) = \phi(\mathbf{FR},\theta) \qquad \forall\, \mathbf{R} \in \mathcal{P}_a, \qquad \forall\, \theta \in \Theta.$

The assumption of frame indifference ensures that rigid body rotations of the crystal do not change the energy. By the Polar Decomposition Theorem[13], any tensor $\mathbf{F}$ with $\det \mathbf{F} > 0$ can be written uniquely as a product of a rotation $\mathbf{Q}$ and a positive-definite symmetric tensor $\mathbf{U}$, i.e,

$$\mathbf{F} = \mathbf{QU} \qquad \text{where } \mathbf{U} = \sqrt{\mathbf{F}^T\mathbf{F}} \qquad \text{and } \mathbf{Q} = \mathbf{FU}^{-1} \in SO(3). \qquad (2.2)$$

Therefore, frame indifference implies that the energy depends only on the positive-definite symmetric part of the deformation gradient. The choice of $\mathcal{P}_a$ as the material symmetry group is

motivated by the molecular theory and reflects the fact that the austenite lattice contains cystallographically indistinguishable directions.

We assume that there is a point group $\mathcal{P}_m \subset \mathcal{P}_a$ associated with the lattice of the martensite which leaves the martensite lattice unchanged. Simple molecular arguments imply that $\mathbf{S}_1$ satisfies

$$\mathbf{R}^T\mathbf{S}_1^T\mathbf{S}_1\mathbf{R} = \mathbf{S}_1^T\mathbf{S}_1 \qquad \forall \qquad \mathbf{R} \in \mathcal{P}_m.$$

It is not generally true that $\mathbf{R}^T\mathbf{S}_1^T\mathbf{S}_1\mathbf{R} = \mathbf{S}_1^T\mathbf{S}_1$ for $\mathbf{R} \in \mathcal{P}_a$. Let $\mathbf{S}_1, \mathbf{S}_2, ..., \mathbf{S}_\nu$ be the distinct tensors of the form $\mathbf{R}^T\mathbf{S}_1\mathbf{R}$ for $\mathbf{R} \in \mathcal{P}_a$. It is easy[66] to see that

$$\nu = \frac{\text{Order of } \mathcal{P}_a}{\text{Order of } \mathcal{P}_m}. \tag{2.3}$$

The configurations described by the deformations $\mathbf{y}(\mathbf{x}) = \mathbf{S}_K\mathbf{x}$ where $K = 1, 2, ..., \nu$ correspond to the different variants of martensite. An immediate consequence of the invariance assumption is that each of these configurations has the same energy.

Above the transformation temperature θ_o, a crystal with no loads applied on it is in the austenite phase. Below θ_o, it is in the martensite phase. At θ_o, there is an exchange of stability and we are led to assume that both the homogeneous austenite as well as homogeneous martensite minimize the energy. Without any loss of generality, we assume that the value at the minimum is zero. Therefore, using the invariance, we conclude that $\phi(\mathbf{F},\theta_o)$ is minimized at the

Austenite well: $\mathcal{A} \stackrel{\text{def}}{=} \{\mathbf{Q} \mid \mathbf{Q} \in SO(3)\}$ and (2.4)

Martensite wells: $\mathcal{M} \stackrel{\text{def}}{=} \bigcup_{K=1}^{\nu} \{\mathbf{Q}\mathbf{S}_K \mid \mathbf{Q} \in SO(3)\}.$

Finally, we assume that the tensors belonging the wells $\mathcal{A}$ and $\mathcal{M}$ are the only minimizers of $\phi(\mathbf{F},\theta_o)$. Therefore, at the transformation temperature, the free energy satisfies

$$0 = \phi(\mathbf{G},\theta_o) < \phi(\mathbf{F},\theta_o) \qquad \forall\, \mathbf{G} \in \mathcal{A}\cup\mathcal{M} \text{ and } \quad \forall\, \mathbf{F} \in \mathcal{D}\setminus\mathcal{A}\cup\mathcal{M}. \tag{2.5}$$

For a energy function described above, it is possible that for certain prescribed boundary conditions there are no minimizers[39]. This may occur even for "acceptable boundary conditions" for which there are functions $\mathbf{y} \in \mathcal{S}$ that satisfy $\mathbf{y} = \mathbf{y}_o$ on $\partial\Omega$. In such cases there is no function $\mathbf{z} \in \mathcal{S}$ that satisfies $\mathbf{z} = \mathbf{y}_o$ on $\partial\Omega$ and for which

$$\mathcal{E}_\Omega[z,\theta_o] \quad = \quad \inf_{\substack{y \in \mathcal{S} \\ y = y_o \text{ on } \partial\Omega}} \mathcal{E}_\Omega[y,\theta_o] \ .$$

However, it is always possible to find a sequence of deformations $y^k \in \mathcal{S}$ which satisfy the prescribed boundary condition and for which $\mathcal{E}_\Omega[y^k,\theta_o]$ becomes smaller and smaller, going to the infimum in the limit. These sequences may not converge in $W^{1,\infty}(\Omega\ ;\ \mathbb{R}^3)$. However, $\nabla y^k \in \mathcal{D}$, a bounded set, and $\|\nabla y^k\|_\infty$ is uniformly bounded independent of k. Hence, $\|y^k\|_{1,\infty}$ is uniformly bounded and by extracting a subsequence if necessary, the sequence converges weak* in $W^{1,\infty}(\Omega\ ;\ \mathbb{R}^3)$ as $k \to \infty$ (denoted by $y^k \overset{*}{\rightharpoonup} y$ in $W^{1,\infty}(\Omega\ ;\ \mathbb{R}^3)$)[20,30]. These sequences of deformations often involve certain microstructure on a finer and finer scale. The fundamental hypothesis of Ball and James[9,10] is that these weak* convergent minimizing sequences model the coherent fine scale microstructure. Recall the following definitions.

A sequence $F^k \overset{*}{\rightharpoonup} F$ in $L^\infty(\Omega\ ;\ \mathbb{R}^m)$ as $k \to \infty$ means that there exists a constant α such that

$$\| F^k \|_\infty \ \le \alpha \qquad \forall \text{ integers } k \qquad \text{and}$$

$$\int_{\Omega'} F^k(x)\, dx \to \int_{\Omega'} F(x)\, dx \quad \forall \text{ smooth subdomains } \Omega' \subset \Omega \text{ as } k \to \infty.$$

A sequence $y^k \overset{*}{\rightharpoonup} y$ in $W^{1,\infty}(\Omega\ ;\ \mathbb{R}^3)$ as $k \to \infty$ means that

$$\nabla y^k \overset{*}{\rightharpoonup} \nabla y \qquad \text{in } L^\infty(\Omega\ ;\ \mathbb{R}^9) \text{ as } k \to \infty \qquad \text{and}$$

$$y^k \to y \qquad \text{uniformly on } \Omega \text{ as } k \to \infty\ .$$

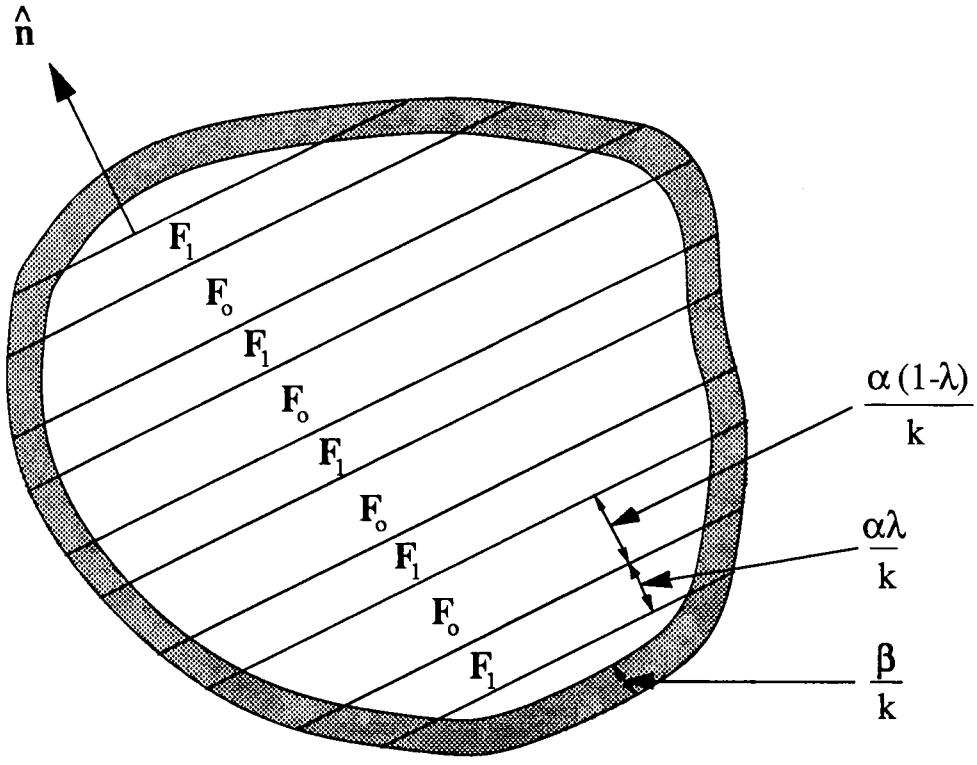

Figure 2.1: The kth term of the sequence of deformations (2.8) involving one level of laminates.

Here is an example of a weak* convergent sequence that satisfies homogeneous boundary conditions.

Example 2.1. (Laminates or Fine Twins) Suppose the tensors $\mathbf{F}_o$ and $\mathbf{F}_1$ satisfy

$$\mathbf{F}_1 - \mathbf{F}_o = \mathbf{a} \otimes \hat{\mathbf{n}} \tag{2.6}$$

for some vector $\mathbf{a}$ and some unit vector $\hat{\mathbf{n}}$. This is the Hadamard jump condition that is necessary and sufficient for constructing any continuous piecewise affine deformation with gradients $\mathbf{F}_o$ and $\mathbf{F}_1$[9,13]. In any such deformation, the gradients can jump only along planes with normal $\hat{\mathbf{n}}$. Let k be any positive integer and $\lambda \in (0,1)$. Let $\chi(t):(0,1) \to \mathbb{R}$ be the characteristic function of $(0,\lambda)$. Extend χ periodically with period 1 to $\mathbb{R}$. Then the deformation

$$\mathbf{z}^k(\mathbf{x}) = \mathbf{F}_o\mathbf{x} + \frac{1}{k} \int_0^{k\mathbf{x}\cdot\hat{\mathbf{n}}} \chi(\tau)\, d\tau\ \mathbf{a}$$

is continuous and piecewise affine with gradients $\mathbf{F}_o$ and $\mathbf{F}_1$ in the alternate bands as shown in Figure 2.1. Notice that the thickness of the bands is scaled by $\frac{1}{k}$. However, $\mathbf{z}^k$ does not satisfy homogeneous boundary conditions. This is achieved by introducing a small transition layer (shaded in Figure 2.1) at the boundary. Following Chipot and Kinderlehrer[19], let $\psi^k : \mathbb{R}^3 \to [0,1]$ be a smooth cut-off function with the following properties:

$$\psi^k = \begin{cases} 0 & \text{outside } \Omega \\ 1 & \mathbf{x} \in \Omega \text{ with distance } (\mathbf{x}, \partial\Omega) \geq \frac{\alpha}{k} \end{cases} \tag{2.7}$$

$$| \nabla \psi^k | \leq \frac{2k}{\alpha} \ .$$

Now, the deformation

$$\mathbf{y}^k(\mathbf{x}) = \psi^k(\mathbf{x})\, \mathbf{z}^k(\mathbf{x}) + (1 - \psi^k(\mathbf{x}))\, \mathbf{F}_\lambda\, \mathbf{x} \qquad \mathbf{x} \in \Omega \tag{2.8}$$

$$\text{where } \mathbf{F}_\lambda = \lambda \mathbf{F}_1 + (1-\lambda)\, \mathbf{F}_o.$$

satisfies homogeneous boundary conditions $\mathbf{F}_\lambda \mathbf{x}$. It is laminated except for a small transition layer at the boundary. Moreover, it is easy to verify that

$$\mathbf{y}^k \overset{*}{\rightharpoonup} \mathbf{y} \qquad \text{in } W^{1,\infty}(\Omega\,;\, \mathbb{R}^3) \qquad \text{where } \mathbf{y}(\mathbf{x}) = \mathbf{F}_\lambda \mathbf{x} \quad \mathbf{x} \in \Omega.$$

Thus as $k \to \infty$, $\mathbf{y}^k$ approximates the homogenous deformation $\mathbf{F}_\lambda \mathbf{x}$ uniformly, while its gradients take on the values $\mathbf{F}_o$ and $\mathbf{F}_1$ except in the transition zone, the volume of which goes to zero. We call $\mathbf{F}_\lambda$ the *average deformation gradient of the laminate.*

Notice that

$$\mathcal{E}_\Omega[\mathbf{y}^k, \theta] \quad \to \quad \text{volume}(\Omega)\ \{\ \lambda \phi(\mathbf{F}_1, \theta) + (1-\lambda)\, \phi(\mathbf{F}_o, \theta)\ \} \qquad \text{while}$$

$$\mathcal{E}_\Omega[\mathbf{y}, \theta] \quad = \quad \text{volume}(\Omega)\ \phi(\lambda \mathbf{F}_1 + (1-\lambda)\mathbf{F}_o, \theta)$$

Thus, unless we make additional hypothesis on ϕ, the limit of the energy is not equal to the energy of the limit configuration. □

To determine the conditions under which given tensors satisfy (2.6), we appeal to Ball and James[10].

Proposition 2.1. (Ball and James[10]) *Given tensors* $\mathbf{F}_o$ and $\mathbf{F}$ *with positive determinants, it is possible to solve*

$$\mathbf{QF} - \mathbf{F}_o = \mathbf{a} \otimes \hat{\mathbf{n}} \tag{2.9}$$

for $\mathbf{Q} \in SO(3)$, $\mathbf{a} \neq \mathbf{0}$ *and* $\hat{\mathbf{n}}$ *if and only if* $\mathbf{C} = \mathbf{F}_o^{-T}\,\mathbf{F}^T\,\mathbf{F}\,\mathbf{F}_o^{-1} \neq \mathbf{1}$ *and the ordered eigenvalues* $\lambda_1 \leq \lambda_2 \leq \lambda_3$ *of* $\mathbf{C}$ *satisfy the condition* $\lambda_2 = 1$. *The solutions are given by*

$$\mathbf{a} = \rho\left(\sqrt{\frac{\lambda_3(1-\lambda_1)}{\lambda_3-\lambda_1}}\,\hat{\mathbf{e}}_1 + \kappa \sqrt{\frac{\lambda_1(\lambda_3-1)}{\lambda_3-\lambda_1}}\,\hat{\mathbf{e}}_3 \right) \qquad \textit{and} \tag{2.10}$$

$$\hat{\mathbf{n}} = \frac{\sqrt{\lambda_3} - \sqrt{\lambda_1}}{\rho\sqrt{\lambda_3-\lambda_1}} \left(-\sqrt{1-\lambda_1}\;\mathbf{F}_o^T\hat{\mathbf{e}}_1 + \kappa\sqrt{\lambda_3-1}\;\mathbf{F}_o^T\hat{\mathbf{e}}_3 \right)$$

where $\rho \neq 0$ *is chosen to make* $|\hat{\mathbf{n}}| = 1$, $\kappa = \pm 1$ *and* $\{\hat{\mathbf{e}}_1, \hat{\mathbf{e}}_2, \hat{\mathbf{e}}_3\}$ *is an eigenbasis of* $\mathbf{C}$ *corresponding to the eigenvalues* λ_1, λ_2 *and* λ_3. *For each of these values of* $\mathbf{a}$ *and* $\hat{\mathbf{n}}$, $\mathbf{Q}$ *is determinted by substituting back in* (2.9). □

Remark 2.1. In the special case when $\mathbf{F}_o$ and $\mathbf{F}$ satisfy

$$\mathbf{F} = \mathbf{R}\mathbf{F}_o\mathbf{R} \qquad \text{for some } \mathbf{R} = \mathbf{R}[180, \hat{\mathbf{e}}] \in \mathcal{P}_a \tag{2.11}$$

($\mathbf{R}$ is a 180° rotation about $\hat{\mathbf{e}}$ and is given by the formula $\mathbf{R} = -\mathbf{1} + 2\,\hat{\mathbf{e}} \otimes \hat{\mathbf{e}}$), it is easy to verify directly that it is always possible to solve (2.9) and that the solutions are given by

(i) $\mathbf{a} = 2\left(\dfrac{\mathbf{F}_o^{-T}\hat{\mathbf{n}}}{|\mathbf{F}_o^{-T}\hat{\mathbf{n}}|^2} - \mathbf{F}_o\hat{\mathbf{n}} \right)$, $\qquad \hat{\mathbf{n}} = \hat{\mathbf{e}}$, $\qquad$ and $\qquad$ (2.12)

(ii) $\mathbf{a} = \rho\,\mathbf{F}_o\hat{\mathbf{e}}$, $\qquad \hat{\mathbf{n}} = \dfrac{2}{\rho}\left(\hat{\mathbf{e}} - \dfrac{\mathbf{F}_o^T\mathbf{F}_o\hat{\mathbf{e}}}{|\mathbf{F}_o\hat{\mathbf{e}}|^2} \right)$. □

The simple example of laminates (2.8) shows that for a sequence that converges weak* in $W^{1,\infty}(\Omega\,;\,\mathbb{R}^3)$, though the deformations converge uniformly, the gradients oscillate and need not converge even pointwise. Thus, if $\mathbf{y}^k \overset{*}{\rightharpoonup} \mathbf{y}$ in $W^{1,\infty}(\Omega\,;\,\mathbb{R}^3)$, it is not true in general that

$$\psi(\nabla \mathbf{y}^k(\mathbf{x})) \overset{*}{\rightharpoonup} \psi(\nabla \mathbf{y}(\mathbf{x})) \qquad \text{in } L^\infty(\Omega\,;\,\mathbb{R}^s) \tag{2.13}$$

for any continuous $\psi:\mathbb{R}^9 \to \mathbb{R}^s$. However, $\nabla \mathbf{y}^k$ is uniformly bounded in $L^\infty(\Omega\,;\,\mathbb{R}^9)$. Consequently, $\psi(\nabla \mathbf{y}^k)$ is uniformly bounded in $L^\infty(\Omega\,;\,\mathbb{R}^s)$ and it contains at least a weak* convergent subsequence. To determine this weak* limit, we need some knowledge of the oscillation of the gradients. The Young measure serves as an accounting device for these oscillations. Here, we state a suitable version of the Young measure theorem.

Theorem 2.1. (The Young Measure Theorem (Ball[7])) *Suppose* $\mathbf{F}^k \overset{*}{\rightharpoonup} \mathbf{F}$ *in* $L^\infty(\Omega\,;\,\mathbb{R}^m)$ *as* $k \to \infty$. *Let* $\mathcal{K} \subset \mathbb{R}^m$ *be compact. Suppose further that for any open* $\mathcal{U} \supset \mathcal{K}$

$$\lim_{k\to\infty} \quad \text{meas } \{\, \mathbf{x} \in \Omega \mid \mathbf{F}^k(\mathbf{x}) \notin \mathcal{U} \,\} = 0.$$

Then, there exists a subsequence, which is also called $\{\mathbf{F}^k\}$, *and a family of probability measures* $\nu_{\mathbf{x}}$ *for* $\mathbf{x} \in \Omega$ *such that*

(i) $\text{supp } \nu_{\mathbf{x}} \subset \mathcal{K}$ *for almost every* $\mathbf{x} \in \Omega$ *and*

(ii) $\psi(\mathbf{F}^k(\mathbf{x})) \overset{*}{\rightharpoonup} \displaystyle\int_{\mathbb{R}^m} \psi(\mathbf{A})\, d\nu_{\mathbf{x}}(\mathbf{A})$ *in* $L^\infty(\Omega\,;\,\mathbb{R}^s)$ *as* $k \to \infty$

for every continuous $\psi:\mathbb{R}^m \to \mathbb{R}^s$. □

For a sequence of deformations, $\mathbf{y}^k \overset{*}{\rightharpoonup} \mathbf{y}$ in $W^{1,\infty}(\Omega\,;\,\mathbb{R}^3)$, let $\nu_{\mathbf{x}}[\{\mathbf{y}^k\}]$ denote the Young measure associated with the sequence of deformation gradients $\mathbf{F}^k = \nabla \mathbf{y}^k$. We will call it the *Young measure of the microstructure.* $\nu_{\mathbf{x}}[\{\mathbf{y}^k\}]$ contains information about the distribution of the gradients $\nabla \mathbf{y}^k$ in the neighborhood of the point $\mathbf{x}$ as $k \to \infty$. For the laminate (2.8) in Example 2.1, it is easy to verify that the Young measure is $\lambda\, \delta_{\mathbf{F}_1} + (1-\lambda)\, \delta_{\mathbf{F}_o}$, where $\delta_{\mathbf{F}}$ is a Dirac mass supported at $\mathbf{F}$. Given any sequence of deformations $\{\mathbf{y}^k\} \subset \mathcal{S}$ which converges weak* in $W^{1,\infty}(\Omega\,;\,\mathbb{R}^3)$, it is possible to calculate the limit energy with a knowledge of the Young measure of the microstucture. Since $\phi(\cdot,\theta_o) : \mathcal{D} \to \mathbb{R}$ is continuous,

$$\lim_{k\to\infty} \mathcal{E}_\Omega[\mathbf{y}^k,\theta_o] = \lim_{k\to\infty} \int_\Omega \phi(\nabla\mathbf{y}^k(\mathbf{x}),\theta_o)\, d\mathbf{x} = \int_\Omega \int_{\mathbb{R}^9} \phi(\mathbf{A},\theta_o)\, d\nu_{\mathbf{x}}(\mathbf{A})\, d\mathbf{x} \qquad (2.14)$$

where $\nu_{\mathbf{x}} = \nu_{\mathbf{x}}[\{\mathbf{y}^k\}]$. Because of our assumptions on ϕ, $\lim_{k\to\infty} \mathcal{E}_\Omega[\mathbf{y}^k,\theta] = 0$ if and only if supp $\nu_{\mathbf{x}} \subset \mathcal{A}\cup\mathcal{M}$ for a.e. $\mathbf{x}\in\Omega$. In particular, the laminate (2.8) has zero limit energy if and only if $\mathbf{F}_o, \mathbf{F}_1 \in \mathcal{A}\cup\mathcal{M}$.

Though (2.13) is not true in general, it does hold for the minors of the matrix[10,20,30]. This is the well-known weak continuity of the minors. The minors of a matrix are its subdeterminants. In three dimensions, the minors are the matrix itself, the cofactor (i.e., the matrix of all 2x2 subdeterminants) and the determinant. Thus, combining (2.13) with the Young measure theorem, we obtain the following theorem.

Theorem 2.2. (The Minors Relations (Ball and James[10])) *Suppose* $\mathbf{y}^k \overset{*}{\rightharpoonup} \mathbf{y}$ *in* $W^{1,\infty}(\Omega\,;\mathbb{R}^3)$ *as* $k\to\infty$. *Let* $\nu_{\mathbf{x}} = \nu_{\mathbf{x}}[\{\mathbf{y}^k\}]$ *be the Young measure of the microstructure.*

Then,

$$\text{(i)}\quad \nabla\mathbf{y}(\mathbf{x}) = \int_{\mathbb{R}^9} \mathbf{A}\, d\nu_{\mathbf{x}}(\mathbf{A})$$

$$\text{(ii)}\quad \operatorname{cof}\nabla\mathbf{y}(\mathbf{x}) = \int_{\mathbb{R}^9} \operatorname{cof}\mathbf{A}\, d\nu_{\mathbf{x}}(\mathbf{A}) \qquad \textit{and} \qquad (2.15)$$

$$\text{(iii)}\quad \det\nabla\mathbf{y}(\mathbf{x}) = \int_{\mathbb{R}^9} \det\mathbf{A}\, d\nu_{\mathbf{x}}(\mathbf{A}) \qquad \textit{for almost every } \mathbf{x}\in\Omega. \qquad \square$$

We now wish to specialize these relations for the special case of homogeneous boundary conditions. In such cases, we can think of an averaged Young measure, which contains information about the distribution of gradients in the the entire domain. This follows from the following theorem.

Theorem 2.3. (The Averaged Young Measure Theorem (Kinderlehrer and Pedregal[40], Ball and Murat[11]) *Suppose* Ω_1 *and* Ω_2 *are open, connected and bounded domains in* $\mathbb{R}^3$ *such that* $\partial\Omega_1$ *and* $\partial\Omega_2$ *are Lipschitz. Suppose* $\mathbf{y}^k \overset{*}{\rightharpoonup} \mathbf{y}$ *in* $W^{1,\infty}(\Omega_1 ; \mathbb{R}^3)$ *as* $k \to \infty$ *and* $\mathbf{y}^k(\mathbf{x}) = \mathbf{F}_o\mathbf{x}$ *on* $\partial\Omega_1$ *for fixed* $\mathbf{F}_o$. *Let* $\nu_{\mathbf{x}} = \nu_{\mathbf{x}}[\{\mathbf{y}^k\}]$ *and suppose* supp $\nu_{\mathbf{x}} \subset \mathcal{K}$.

Then, there exists a sequence $\mathbf{z}^k \overset{*}{\rightharpoonup} \mathbf{z}$ *in* $W^{1,\infty}(\Omega_2 ; \mathbb{R}^3)$ *as* $k \to \infty$ *such that* $\nu_{\mathbf{x}}[\{\mathbf{z}^k\}]$ *is independent of* $\mathbf{x}$. *i.e.,* $\nu_{\mathbf{x}}[\{\mathbf{z}^k\}] = \mu$. *Moreover,*

$$\begin{aligned}
&\text{(i)} && \operatorname{supp}\mu \subset \mathcal{K} \\
&\text{(ii)} && \mathbf{z}^k(\mathbf{x}) = \mathbf{F}_o\mathbf{x} && \mathbf{x} \in \partial\Omega_2 && \textit{for every } k, \qquad (2.16)\\
&\text{(iii)} && \mathbf{z}(\mathbf{x}) = \mathbf{F}_o\mathbf{x} && \mathbf{x} \in \Omega_2, && \textit{and}
\end{aligned}$$

$$\text{(iv)} \qquad \int_{\mathbb{R}^9} \psi(\mathbf{A})\, d\mu(\mathbf{A}) = \frac{1}{\text{volume}(\Omega_1)} \int_{\Omega_1} \int_{\mathbb{R}^9} \psi(\mathbf{A})\, d\nu_{\mathbf{x}}(\mathbf{A})\, d\mathbf{x}$$

for every continuous $\psi:\mathbb{R}^9 \to \mathbb{R}^s$. □

We will call any microstructure homogeneous if its Young measure is independent of $\mathbf{x}$. The theorem tells us that if there is a microstructure which satisfies homogeneous boundary conditions in one domain, it is possible to find (construct) a homogeneous microstructure on any other domain that satisfies the same boundary conditions. Moreover, the Young measures of both microstructures have the same support. Therefore, in problems with homogeneous boundary conditions, we can pick any suitable domain and consider only homogeneous microstructures.

Given $\mathbf{y}^k \overset{*}{\rightharpoonup} \mathbf{y}$ in $W^{1,\infty}(\Omega ; \mathbb{R}^3)$, we set $\Omega_1 = \Omega_2 = \Omega$. We call the Young measure $\mu[\{\mathbf{y}^k\}]$ delivered by the above theorem the *averaged Young measure of the microstructure.* It contains information about the distribution of gradients in the entire domain.

The minors are also null Lagrangians[22]. Thus, their integrals depends only on the boundary values. In particular, for a deformation $\mathbf{y}$ satisfying homogeneous boundary condition $\mathbf{y}(\mathbf{x}) = \mathbf{F}_o\mathbf{x}$ on $\partial\Omega$,

$$\int_{\Omega} \psi(\nabla\mathbf{y}(\mathbf{x}))\, d\mathbf{x} = \psi(\mathbf{F}_o)\ \text{volume}(\Omega). \qquad (2.17)$$

for any minor ψ. Therefore, integrating the minors relations (2.15) over Ω, and using (2.17) along with (2.16)(iv) for the averaged Young measure, we obtain the following.

Theorem 2.4. (The Minors Relations for Homogeneous Boundary Conditions) *Suppose* $y^k \overset{*}{\rightharpoonup} y$ *in* $W^{1,\infty}(\Omega\,;\,\mathbb{R}^3)$ *as* $k \to \infty$ *and* $y^k(x) = F_o x$ *on* $\partial\Omega$ *for fixed* F_o *and suppose that* $\mu = \mu[\{y^k\}]$ *is the averaged Young measure.*

Then, (i) $F_o = \int_{\mathbb{R}^9} A \, d\mu(A)$,

$$\text{(ii) } \operatorname{cof} F_o = \int_{\mathbb{R}^9} \operatorname{cof} A \, d\mu(A) \qquad \textit{and} \tag{2.18}$$

$$\text{(iii) } \det F_o = \int_{\mathbb{R}^9} \det A \, d\mu(A). \qquad \square$$

For the laminate (2.8) in Example 2.1, (2.18) reduces to

$$\begin{aligned} &\operatorname{cof}(\lambda F_1 + (1-\lambda) F_o) = \lambda \operatorname{cof} F_1 + (1-\lambda) \operatorname{cof} F_o \\ &\det(\lambda F_1 + (1-\lambda) F_o) = \lambda \det F_1 + (1-\lambda) \det F_o \end{aligned} \tag{2.19}$$

for F_o and F_1 which satisfy (2.6) and $\lambda \in [0,1]$.

Before we proceed, we construct one more weak* convergent sequence which is use repeatedly in Section 3 in order to show sufficiency. Given any microstructure that satisfies homogeneous boundary conditions, the averaged Young measure theorem delivers a homogeneous microstructure. Under suitable hypothesis, it is possible to construct a sequence of laminates consisting of alternating bands of two such microstructures.

Example 2.2. (Multilaminates) Suppose

$$\mathbf{y}^k \overset{*}{\rightharpoonup} \mathbf{y} \text{ in } W^{1,\infty}(\Omega\,;\,\mathbb{R}^3),\ \mathbf{y}^k(\mathbf{x}) = \mathbf{F}_o\mathbf{x} \text{ on } \partial\Omega \text{ and supp } \mu[\{\mathbf{y}^k\}] \subset \mathcal{K}_o \quad \text{and}$$

$$\mathbf{z}^k \overset{*}{\rightharpoonup} \mathbf{z} \text{ in } W^{1,\infty}(\Omega\,;\,\mathbb{R}^3),\ \mathbf{z}^k(\mathbf{x}) = \mathbf{F}_1\mathbf{x} \text{ on } \partial\Omega \text{ and supp } \mu[\{\mathbf{z}^k\}] \subset \mathcal{K}_1$$

where $\mathbf{F}_1 - \mathbf{F}_o = \mathbf{a} \otimes \hat{\mathbf{n}}$ for some vectors $\mathbf{a}$ and $\hat{\mathbf{n}}$. For any $\lambda \in [0,1]$, set $\mathbf{F}_\lambda = \lambda\mathbf{F}_1 + (1-\lambda)\mathbf{F}_o$. Then, it is possible to find a sequence of deformations $\mathbf{w}^k$ such that

$$\begin{aligned} &\mathbf{w}^k \overset{*}{\rightharpoonup} \mathbf{w} \quad \text{in } W^{1,\infty}(\Omega\,;\,\mathbb{R}^3) \qquad \text{where } \mathbf{w}(\mathbf{x}) = \mathbf{F}_\lambda\mathbf{x} \quad \mathbf{x} \in \Omega. \\ &\mathbf{w}^k(\mathbf{x}) = \mathbf{F}_\lambda\mathbf{x} \qquad\qquad \mathbf{x} \in \partial\Omega \qquad\qquad \text{and} \qquad\qquad (2.20) \\ &\text{supp } \mu[\{\mathbf{w}^k\}] \subset \mathcal{K}_o \cup \mathcal{K}_1. \end{aligned}$$

Here is a sketch of the construction. Firstly, according to the averaged Young measure theorem, we may assume without any loss of generality that

$$\mathbf{y}(\mathbf{x}) = \mathbf{F}_o\mathbf{x} \quad \text{and} \quad \mathbf{z}(\mathbf{x}) = \mathbf{F}_1\mathbf{x} \qquad \mathbf{x} \in \Omega.$$

For each positive integer j, set $\beta^j = \max\{ \sup_{x\in\Omega} |\, \mathbf{y}^j(\mathbf{x}) - \mathbf{y}(\mathbf{x})\,|,\ \sup_{x\in\Omega} |\, \mathbf{z}^j(\mathbf{x}) - \mathbf{z}(\mathbf{x})\,| \}$. Since $\mathbf{y}^j$ and $\mathbf{z}^j$ converge uniformly on Ω, $\beta^j \to 0$ as $j \to \infty$. For positive integers j and k with j sufficiently large, find smooth functions $\Psi^{k,j} : [0, \frac{1}{k}] \to [0, 1]$ such that

$$\Psi^{k,j}(\tau) = \begin{cases} 0 & \tau = 0,\ \frac{\lambda}{k},\ \frac{1}{k} \\ \\ 1 & \tau \in [\beta^j,\ \frac{\lambda}{k} - \beta^j] \cup [\frac{\lambda}{k} + \beta^j,\ \frac{1}{k} - \beta^j] \end{cases} \qquad \text{and}$$

$$\left|\frac{d\Psi^{k,j}}{d\tau}\right| \le \frac{2}{\beta^j}\,.$$

Extend $\Psi^{k,j}$ periodically with period $\frac{1}{k}$ to $\mathbb{R}$. Define the function $\mathbf{u}^{k,j}(\mathbf{x}) : \Omega \to \mathbb{R}^3$ by

$$\mathbf{u}^{k,j}(\mathbf{x}) = \begin{cases} \Psi^{k,j}(\mathbf{x}\cdot\hat{\mathbf{n}})\,\mathbf{z}^j(\mathbf{x}) + (1-\Psi^{k,j}(\mathbf{x}\cdot\hat{\mathbf{n}}))\mathbf{F}_1\mathbf{x} - \frac{i\,(1-\lambda)}{k}\,\mathbf{a} & \frac{i}{k} < \mathbf{x}\cdot\hat{\mathbf{n}} \le \frac{i+\lambda}{k} \\ \\ \Psi^{k,j}(\mathbf{x}\cdot\hat{\mathbf{n}})\,\mathbf{y}^j(\mathbf{x}) + (1-\Psi^{k,j}(\mathbf{x}\cdot\hat{\mathbf{n}}))\mathbf{F}_o\mathbf{x} + \frac{(i+1)\,\lambda}{k}\,\mathbf{a} & \frac{i+\lambda}{k} < \mathbf{x}\cdot\hat{\mathbf{n}} \le \frac{i+1}{k} \end{cases}$$

for $\mathbf{x} \in \Omega$ and integers i. It is easy to verify that $\mathbf{u}^{k,j} \in W^{1,\infty}(\Omega\,;\,\mathbb{R}^3)$.

Let smooth cut-off functions $\psi^k : \mathbb{R}^3 \to [0,1]$ satisfy (2.7). Set,

$$\mathbf{w}^{k,j}(\mathbf{x}) = \psi^k(\mathbf{x})\,\mathbf{u}^{k,j}(\mathbf{x}) + (1 - \psi^k(\mathbf{x}))\,\mathbf{F}_\lambda \mathbf{x} \qquad \mathbf{x} \in \Omega \qquad \text{where } \mathbf{F}_\lambda = \lambda \mathbf{F}_1 + (1-\lambda)\,\mathbf{F}_o\,.$$

Find J(k) such that $\beta^{J(k)}\, k \to 0$ as $k \to \infty$ (for example, $\beta^{J(k)} \le \frac{1}{k^2}$). This is possible since $\beta^j \to 0$.

Set $\mathbf{w}^k(\mathbf{x}) = \mathbf{w}^{k,J(k)}(\mathbf{x}) \qquad \mathbf{x} \in \Omega.$

It is a matter of analysis to verify that $\mathbf{w}^k$ satisfies (2.20). We call $\mathbf{F}_\lambda$ the *average deformation gradient of the multilaminate.* □

Given two laminates, each of the form (2.8), we may follow the above construction to obtain a multilaminate which resembles Figure 2.2. We call this a laminate with two levels or a double laminate. Using the same construction on two double laminates, we may obtain a laminate with three levels or a triple laminate. Proceeding similarly, we may obtain a laminate with n levels. To make the jargon complete, we call the laminate (2.8) a single laminate or a laminate with one level.

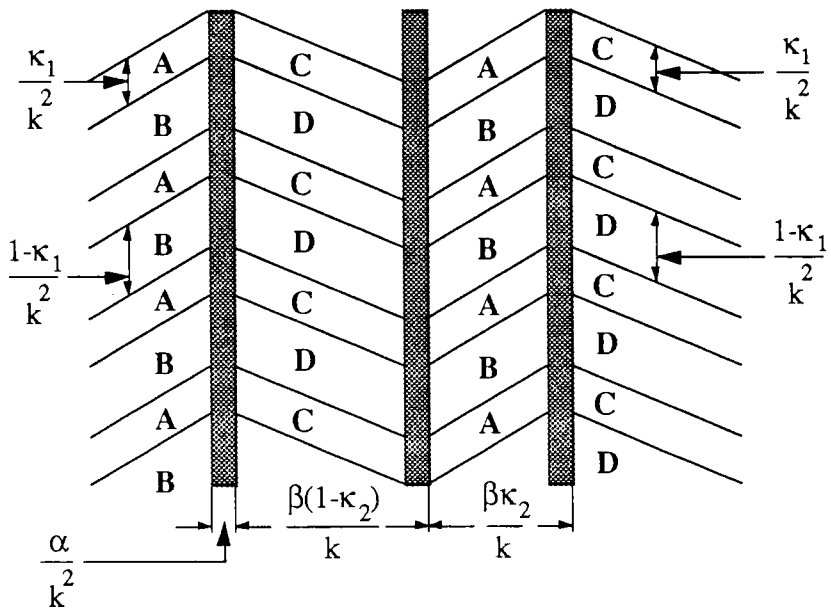

Figure 2.2: The kth term of the sequence of deformations involving two levels of laminates.

§3. SELF-ACCOMMODATION

In this section, we ask which materials are able to form a self-accommodating microstructure. Since $\mathbf{S}_1$ can be measured for a given material, we want to find necessary and sufficient conditions on $\mathbf{S}_1$ that there exist a self-accommodating microstructure. A self-accommodating microstructure consists of martensitic variants arranged in such a manner that the boundary of the crystal suffers suffers no deformation. Recall that we have chosen SO(3)**1** to correspond to the austenite (2.4). Since minimizing sequences model microstructure, we adopt the following definition.

A *self-accommodating microstructure* is a sequence of deformations $\{\mathbf{y}^k\} \subset \mathcal{S}$ which converges weak* in $W^{1,\infty}(\Omega\,;\,\mathbb{R}^3)$ and satisfies

$$\mathbf{y}^k(\mathbf{x}) = \mathbf{x} \qquad \mathbf{x} \in \partial\Omega \qquad \text{and} \qquad (3.1)$$

$$\text{supp } \nu_{\mathbf{x}}[\{\mathbf{y}^k\}] \subset \mathcal{M} \qquad \text{for almost every } \mathbf{x} \in \Omega,$$

Recall that $\nu_{\mathbf{x}}[\{\mathbf{y}^k\}]$ is the Young measure of the microstructure. It follows from (2.14) that for this sequence $\mathcal{E}_\Omega[\mathbf{y}^k,\theta_o] \to 0$ as $k \to \infty$.

The necessary and sufficient condition for self-accommodation are summarized in Table 3.1. Though the ideas are the same, it is necessary to study the problem case by case. The necessity of the conditions in Table 3.1 will be derived using the minors relations for homogeneous boundary condition (Theorem 2.4). In each case, the sufficiency of the conditions listed in Table 3.1 will be demonstrated by constructing self-accommodating microstructures.

In order to save a few words, we say that a tensor $\mathbf{F}$ is *achieved* if there is a sequence of deformations $\{\mathbf{y}^k\} \subset \mathcal{S}$ which converges weak* in $W^{1,\infty}(\Omega\,;\,\mathbb{R}^3)$ and satisfies

$$\mathbf{y}^k(\mathbf{x}) = \mathbf{F}\mathbf{x} \quad \mathbf{x} \in \partial\Omega \qquad \text{and} \qquad \text{supp } \nu_{\mathbf{x}}[\{\mathbf{y}^k\}] \subset \mathcal{M} \quad \text{for almost every } \mathbf{x} \in \Omega.$$

For example, if we have a self-accommodating microstructure, we say that **1** is achieved.

Table 3.1: Necessary and sufficient conditions for self-accommodation

Group $\mathcal{P}_a$ (Symmetry of the austenite)	Necessary and Sufficient conditions for self-accommodation
Cubic	$\det \mathbf{S}_1 = 1$
Tetragonal	(i) $\det \mathbf{S}_1 = 1$ and (ii) $\frac{1}{E_{22}E_{33} - E_{23}^2} \leq 1 \leq E_{11}$
Orthorhombic	(i) $\det \mathbf{S}_1 = 1$, (ii) $\frac{1}{E_{22}E_{33} - E_{23}^2} \leq 1 \leq E_{11}$, (iii) $\frac{1}{E_{11}E_{33} - E_{13}^2} \leq 1 \leq E_{22}$ and (iv) $\frac{1}{E_{11}E_{22} - E_{12}^2} \leq 1 \leq E_{33}$.
Monoclinic	The two well problem. (See Section 3.4 and [10])

$\mathbf{S}_1$ is the the transformation strain and $\mathbf{E} = \mathbf{S}_1^T\mathbf{S}_1$. The components of $\mathbf{E}$ are expressed in an orthonormal basis parallel to the cubic/tetragonal/orthorhombic unit cell of the austenite. In the case of the tetragonal austenite, $\hat{\mathbf{i}}_1$ is the "c-axis" of the tetragonal lattice.

Before giving the proofs, we make a few remarks.

Remark 3.1. If $\mathbf{F}$ is achieved, $\det \mathbf{F} = \det \mathbf{S}_1$. Notice that for every $\mathbf{A} \in \mathcal{M}$, $\det \mathbf{A} = \det \mathbf{S}_1$. Therefore, by the minors relations for homogeneous boundary conditions (2.18)(iii),

$$\det \mathbf{F} = \int_{\mathcal{M}} \det \mathbf{A}\, d\mu(\mathbf{A}) = \int_{\mathcal{M}} \det \mathbf{S}_1\, d\mu(\mathbf{A}) = \det \mathbf{S}_1. \qquad \square$$

Remark 3.2. Suppose $\mathbf{F}$ is achieved. Then, for any $\mathbf{Q} \in SO(3)$ and any $\mathbf{R} \in \mathcal{P}_a$, $\mathbf{QFR}$ is achieved. This follows from the invariance of the set $\mathcal{M}$. In particular, $\sqrt{\mathbf{C}}$, where $\mathbf{C} = \mathbf{F}^T\mathbf{F}$, is achieved. This is a consequence of the Polar Decomposition Theorem (2.2). $\square$

Remark 3.3. Suppose $\mathbf{F}_o$ and $\mathbf{F}_1$ are achieved where $\mathbf{F}_1 - \mathbf{F}_o = \mathbf{a} \otimes \hat{\mathbf{n}}$ for some vectors $\mathbf{a}$ and $\hat{\mathbf{n}}$. Then, for any $\lambda \in [0,1]$, $\mathbf{F}_\lambda = \lambda\mathbf{F}_1 + (1-\lambda)\mathbf{F}_o$ is achieved. This follows by constructing multilaminates as described in Section 2 (Example 2.2). Notice that we may write, $\mathbf{F}_\lambda = \mathbf{F}_o + \lambda\, \mathbf{a} \otimes \hat{\mathbf{n}}$ and

$$\mathbf{C}_\lambda = \mathbf{F}_\lambda^T\mathbf{F}_\lambda = \mathbf{F}_o^T\mathbf{F}_o + \lambda(\mathbf{F}_o^T\mathbf{a} \otimes \hat{\mathbf{n}} + \hat{\mathbf{n}} \otimes \mathbf{F}_o^T\mathbf{a}) + \lambda^2 |\mathbf{a}|^2 \hat{\mathbf{n}} \otimes \hat{\mathbf{n}}, \qquad (3.2)$$

$$\mathbf{C}_o = \mathbf{F}_o^T\mathbf{F}_o \quad \text{and} \quad \mathbf{C}_1 = \mathbf{F}_1^T\mathbf{F}_1.$$

In particular, if $\mathbf{R} = \mathbf{R}[180,\hat{\mathbf{e}}] \in \mathcal{P}_a$, it follows from Remark 2.1 that for a suitable $\mathbf{Q} \in SO(3)$, $\mathbf{F}_\lambda = \lambda\mathbf{QRF}_o\mathbf{R} + (1-\lambda)\mathbf{F}_o$ is achieved. $\mathbf{F}_\lambda^T\mathbf{F}_\lambda$ is given by (3.2) for $\mathbf{a}$ and $\hat{\mathbf{n}}$ according to (2.12)(i). In this case, $\mathbf{C}_1 = \mathbf{RC}_o\mathbf{R}$. $\square$

Remark 3.4. (Diagonalization about $\hat{\mathbf{i}}_1$) Suppose $\mathbf{F}_o$ is achieved and $\mathbf{R} = \mathbf{R}[180,\hat{\mathbf{i}}_1] \in \mathcal{P}_a$.

If $\mathbf{C}_o = \mathbf{F}_o^T\mathbf{F}_o = \begin{bmatrix} C_{11} & C_{12} & C_{13} \\ C_{12} & C_{22} & C_{23} \\ C_{13} & C_{23} & C_{33} \end{bmatrix}$ in an orthonormal basis $\{\hat{\mathbf{i}}_1, \hat{\mathbf{i}}_2, \hat{\mathbf{i}}_3\}$,

we show that we can achieve $\mathbf{F}$ where $\mathbf{F}^T\mathbf{F}$ has the following form for some positive constant α.

$$\begin{bmatrix} \alpha^2 & 0 & 0 \\ 0 & C_{22} & C_{23} \\ 0 & C_{23} & C_{33} \end{bmatrix} \qquad (3.3)$$

By Remark 3.3, for a suitable $\mathbf{Q} \in SO(3)$, $\mathbf{F}_\lambda = \lambda\mathbf{Q}\mathbf{R}\mathbf{F}_o\mathbf{R} + (1-\lambda)\mathbf{F}_o$ is achieved for any $\lambda \in [0,1]$. By (3.2) and (2.12)(i),

$$\mathbf{C}_\lambda = \mathbf{F}_\lambda^T\mathbf{F}_\lambda = \mathbf{C}_o + \lambda(\mathbf{F}_o^T\mathbf{a} \otimes \hat{\mathbf{i}}_1 + \hat{\mathbf{i}}_1 \otimes \mathbf{F}_o^T\mathbf{a}) + \lambda^2 |\mathbf{a}|^2 \hat{\mathbf{i}}_1 \otimes \hat{\mathbf{i}}_1.$$

$$\mathbf{C}_o = \begin{bmatrix} C_{11} & C_{12} & C_{13} \\ C_{12} & C_{22} & C_{23} \\ C_{13} & C_{23} & C_{33} \end{bmatrix} \quad \text{and} \quad \mathbf{C}_1 = \mathbf{R}\mathbf{C}_o\mathbf{R} = \begin{bmatrix} C_{11} & -C_{12} & -C_{13} \\ -C_{12} & C_{22} & C_{23} \\ -C_{13} & C_{23} & C_{33} \end{bmatrix}.$$

Notice, if $ij \neq 11$, $(\mathbf{C}_\lambda)_{ij} = \hat{\mathbf{i}}_i \cdot \mathbf{C}_\lambda \hat{\mathbf{i}}_j$ is a linear function of λ.

Also, if ij = 12, 21, 31 or 13, $\quad (\mathbf{C}_o)_{ij} = -(\mathbf{C}_1)_{ij}. \quad \Rightarrow \quad (\mathbf{C}_{1/2})_{ij} = 0.$

Similarly, if $i\neq1, j\neq1$ $\quad (\mathbf{C}_o)_{ij} = (\mathbf{C}_1)_{ij}. \quad \Rightarrow \quad (\mathbf{C}_\lambda)_{ij} = (\mathbf{C}_o)_{ij} \quad \forall \ \lambda \in [0,1].$

Therefore, $\mathbf{C}_{1/2}$ = has the form (3.3). □

We can similarly have diagonalization about $\hat{\mathbf{i}}_2$ and diagonalization about $\hat{\mathbf{i}}_3$ provided $\mathbf{R}[180,\hat{\mathbf{i}}_2]$ and $\mathbf{R}[180,\hat{\mathbf{i}}_3]$ belong to $\mathcal{P}_a$ respectively.

3.1. Self-accommodation with Cubic Austenite. We now restrict ourselves to the case when the austenite lattice has cubic symmetry. $\mathcal{P}_a$, the point group of the austenite, is the cubic group - the group of 24 rotations that map a cube back into itself. In an orthonormal basis $\{\hat{\mathbf{i}}_1,\hat{\mathbf{i}}_2,\hat{\mathbf{i}}_3\}$ chosen parallel to sides of the cubic unit cell of the austenite lattice, it consists of the elements

1,

$$\mathbf{R}[\pm90,\hat{\mathbf{i}}_1],\ \mathbf{R}[\pm90,\hat{\mathbf{i}}_2],\ \mathbf{R}[\pm90,\hat{\mathbf{i}}_3], \tag{3.4}$$

$$\mathbf{R}[\pm120,\hat{\mathbf{i}}_1 + \hat{\mathbf{i}}_2 + \hat{\mathbf{i}}_3],\ \mathbf{R}[\pm120,-\hat{\mathbf{i}}_1 + \hat{\mathbf{i}}_2 + \hat{\mathbf{i}}_3],\ \mathbf{R}[\pm120,\hat{\mathbf{i}}_1 - \hat{\mathbf{i}}_2 + \hat{\mathbf{i}}_3],\ \mathbf{R}[\pm120,\hat{\mathbf{i}}_1 + \hat{\mathbf{i}}_2 - \hat{\mathbf{i}}_3],$$

$$\mathbf{R}[180,\hat{\mathbf{i}}_1],\ \mathbf{R}[180,\hat{\mathbf{i}}_2],\ \mathbf{R}[180,\hat{\mathbf{i}}_3],\ \mathbf{R}[180,\hat{\mathbf{i}}_1 \pm \hat{\mathbf{i}}_2],\ \mathbf{R}[180,\hat{\mathbf{i}}_2 \pm \hat{\mathbf{i}}_3] \text{ and } \mathbf{R}[180,\hat{\mathbf{i}}_3 \pm \hat{\mathbf{i}}_1].$$

Without any assumption on the symmetry of the martensite except that $\mathcal{P}_m \subset \mathcal{P}_a$, we will show that the martensite is self-accommodating if and only if the transformation is volume preserving i.e., $\det \mathbf{S}_1 = 1$. All calculations are performed in the orthonormal basis $\{\hat{\mathbf{i}}_1,\hat{\mathbf{i}}_2,\hat{\mathbf{i}}_3\}$.

Necessity. Given any self-accommodating microstructure (3.1), it follows from Remark 3.1 that $\det \mathbf{S}_1 = 1$.

Sufficiency. Assuming that $\det \mathbf{S}_1 = 1$, we now show in two steps that $\mathbf{1}$ is achieved.

Step 1: In this step, we show that Diag$[\alpha,\beta,\gamma]$*, where $\alpha \le \beta \le \gamma$ are positive constants satisfying $\alpha\beta\gamma = 1$, is achieved.

Using the diagonalization procedure about $\hat{\mathbf{i}}_1$ described in Remark 3.4 with $\mathbf{F}_o = \mathbf{S}_1$, we achieve $\mathbf{F}$ where $\mathbf{F}^T\mathbf{F}$ has the form (3.3). Now use diagonalization about $\hat{\mathbf{i}}_2$ to achieve $\mathbf{G}$ where $\mathbf{G}^T\mathbf{G} = \text{Diag}[\alpha^2,\beta^2,\gamma^2]$ where α, β and γ are positive constants. Therefore, appealing to Remark 3.2, Diag$[\alpha,\beta,\gamma]$ is achieved.

Now if $\mathbf{R} = \mathbf{R}[180,\hat{\mathbf{i}}_1 + \hat{\mathbf{i}}_2]$, $\qquad \mathbf{R}\,\text{Diag}[\alpha,\beta,\gamma]\mathbf{R} = \text{Diag}[\beta,\alpha,\gamma]$.

Similarly, using $\mathbf{R}[180,\hat{\mathbf{i}}_2 + \hat{\mathbf{i}}_3]$ and $\mathbf{R}[180,\hat{\mathbf{i}}_1 + \hat{\mathbf{i}}_3]$, it is possible to interchange β with γ and α with γ respectively. Since all these rotations belong to $\mathcal{P}_a$, by Remark 3.2, $\mathbf{U} = \text{Diag}[\alpha,\beta,\gamma]$ with $\alpha \le \beta \le \gamma$ is achieved. By assumption, $\det \mathbf{S}_1 = 1$ and it follows from Remark 3.1 that $\alpha\beta\gamma = 1$. This completes Step 1.

Step 2: Given that $\mathbf{U} = \text{Diag}[\alpha,\beta,\gamma]$, where $\alpha \le \beta \le \gamma$ satisfy $\alpha\beta\gamma = 1$, is achieved, we show in this step that $\mathbf{1}$ is achieved. Without loss of generality, we may assume that $\alpha < 1 < \gamma$. If this does not hold, $\alpha = \beta = \gamma = 1$ and we are done.

Let $\mathbf{R} = \mathbf{R}[180, \hat{\mathbf{i}}_1+\hat{\mathbf{i}}_3]$. $\mathbf{R} \in \mathcal{P}_a$. Therefore, by Remark 3.3 for a suitable $\mathbf{Q} \in SO(3)$ and for any $\lambda \in [0,1]$, it is possible to achieve $\mathbf{F}_\lambda = \lambda\mathbf{QRUR} + (1-\lambda)\mathbf{U}$. From (2.12)(i) and (3.2), it is a long, but easy calculation to see that

$$\mathbf{C}_\lambda = \mathbf{F}_\lambda^T\mathbf{F}_\lambda = \begin{bmatrix} \alpha^2(1-\zeta)^2 + \gamma^2\zeta^2 & 0 & \xi(\lambda) \\ 0 & \beta^2 & 0 \\ \xi(\lambda) & 0 & \alpha^2\zeta^2 + \gamma^2(1+\zeta)^2 \end{bmatrix}$$

$$\text{where } \zeta = \lambda\frac{\alpha^2 - \gamma^2}{\alpha^2 + \gamma^2}.$$

Now, use the diagonalization about $\hat{\mathbf{i}}_1$ to achieve $\mathbf{G}_\lambda$ such that

*Diag$[\alpha,\beta,\gamma]$ denotes the diagonal 3x3 matrix with diagonal elements α, β and γ.

$$G_\lambda^T G_\lambda = \begin{bmatrix} \eta^2(\lambda) & 0 & 0 \\ 0 & \beta^2 & 0 \\ 0 & 0 & \alpha^2\zeta^2 + \gamma^2(1+\zeta)^2 \end{bmatrix}$$

where $\eta(\lambda)$ is some positive function of λ.

The idea now is to pick λ such that $\alpha^2\zeta^2 + \gamma^2(1+\zeta)^2 = 1$. This equation is quadratic in λ with the solution

$$\lambda = \frac{\gamma^2 - \sqrt{\alpha^2 + \gamma^2 - \alpha^2\gamma^2}}{\gamma^2 - \alpha^2} .$$

It is now necessary to verify that $\lambda \in (0,1)$.

Notice that since $\alpha < 1$, $\quad \alpha^2 + \gamma^2 - \alpha^2\gamma^2 - \alpha^4 = (\alpha^2 + \gamma^2)(1 - \alpha^2) > 0$. Therefore,

$\alpha^2 + \gamma^2 - \alpha^2\gamma^2 > \alpha^4 > 0$ and $\sqrt{\alpha^2 + \gamma^2 - \alpha^2\gamma^2}$ is real.

Also, $\sqrt{\alpha^2 + \gamma^2 - \alpha^2\gamma^2} > \alpha^2$ which implies that $\lambda < 1$.

Similarly, since $\gamma > 1$, $\quad \alpha^2 + \gamma^2 - \alpha^2\gamma^2 - \gamma^4 = (\alpha^2 + \gamma^2)(1 - \gamma^2) < 0$. Therefore,

$\alpha^2 + \gamma^2 - \alpha^2\gamma^2 < \gamma^4$ so that $\sqrt{\alpha^2 + \gamma^2 - \alpha^2\gamma^2} < \gamma^2$. This implies that $\lambda > 0$.

Thus for an appropriate choice of λ, $G_\lambda^T G_\lambda = \text{Diag}[\eta^2,\beta^2,1]$. Appealing to Remark 3.2, we achieve $\text{Diag}[\eta,\beta,1]$. But since $\det \mathbf{S}_1 = 1$, $\eta\beta = 1$ and $\eta = \frac{1}{\beta}$. If $\beta \neq 1$, then either $\beta < 1 < \eta$ or $\eta < 1 < \beta$. In either case, it is possible to repeat the same construction again, but with $\mathbf{R}[180,\hat{\mathbf{i}}_1+\hat{\mathbf{i}}_2]$, to achieve **1**.

3.2. Self-accommodation with Tetragonal Austenite. Suppose that $\mathcal{P}_a$, the point group of the austenite, is the tetragonal group consisting of eight rotations. In an orthonormal basis $\{\hat{\mathbf{i}}_1,\hat{\mathbf{i}}_2,\hat{\mathbf{i}}_3\}$ chosen parallel to the sides of the tetragonal cell, $\mathcal{P}_a$ consists of the elements

1,

$$\mathbf{R}[\pm 90,\hat{\mathbf{i}}_1], \tag{3.5}$$

$\mathbf{R}[180,\hat{\mathbf{i}}_1]$, $\mathbf{R}[180,\hat{\mathbf{i}}_2]$, $\mathbf{R}[180,\hat{\mathbf{i}}_3]$ and $\mathbf{R}[180,\hat{\mathbf{i}}_2 \pm \hat{\mathbf{i}}_3]$.

$\hat{\mathbf{i}}_1$ is the "c-axis" of the tetragonal lattice. There is no assumption on the symmetry of the martensite except that $\mathcal{P}_m \subset \mathcal{P}_a$ and $\mathbf{S}_1$ is any tensor with positive determinant. All calculations are performed in the orthonormal basis $\{\hat{\mathbf{i}}_1,\hat{\mathbf{i}}_2,\hat{\mathbf{i}}_3\}$.

Let $\mathbf{E} = \mathbf{S}_1^T\mathbf{S}_1$ and let E_{ij} be the components of $\mathbf{E}$ in the basis $\{\hat{\mathbf{i}}_1,\hat{\mathbf{i}}_2,\hat{\mathbf{i}}_3\}$. Then, the material is self-accommodating if and only if

$$\text{(i)} \quad \det \mathbf{S}_1 = 1 \qquad \text{and} \tag{3.6}$$

$$\text{(ii)} \quad \frac{1}{E_{22}E_{33} - E_{23}^2} \le 1 \le E_{11}.$$

Necessity. Given any self-accommodating microstructure (3.1), we now show that it satisfies (3.6). (3.6)(i) follows from Remark 3.1. To see (3.6)(ii), let μ be the averaged Young measure of the given self-accommodating microstructure. Because supp $\mu \subset \mathcal{M}$, we have from (2.18)(i)

$$\mathbf{1} = \int_{\mathcal{M}} \mathbf{A}\, d\mu(\mathbf{A}), \qquad \text{so that} \qquad \mathbf{e} = \int_{\mathcal{M}} \mathbf{A}\mathbf{e}\, d\mu(\mathbf{A}) \qquad \forall\, \mathbf{e} \in \mathbb{R}^3.$$

According to the Jensen's inequality[70], given any convex function $\psi:\mathbb{R}^m \to \mathbb{R}$ and any probability measure μ with support contained in $\mathcal{K}$,

$$\psi\left(\int_{\mathcal{K}} \mathbf{A}\, d\mu(\mathbf{A}) \right) \le \int_{\mathcal{K}} \psi(\mathbf{A})\, d\mu(\mathbf{A}).$$

Since $|\mathbf{e}|^2$ is convex function,

$$|\mathbf{e}|^2 = \left| \int_{\mathcal{M}} \mathbf{A}\mathbf{e}\, d\mu(\mathbf{A}) \right|^2 \leq \int_{\mathcal{M}} |\mathbf{A}\mathbf{e}|^2\, d\mu(\mathbf{A}) \leq \max_{K=1,..,\nu} \mathbf{e}\cdot\mathbf{S}_K^T\mathbf{S}_K\mathbf{e}.$$

To obtain the last inequality, we use the fact that if $\mathbf{A} \in \mathcal{M}$, $\mathbf{A} = \mathbf{Q}\mathbf{S}_K$ for some K = 1, ..., ν and some $\mathbf{Q} \in SO(3)$.

Set $\mathbf{e} = \hat{\mathbf{i}}_1$. Recall that $\mathbf{S}_K = \mathbf{R}^T\mathbf{S}_1\mathbf{R}$ for some $\mathbf{R} \in \mathcal{P}_a$ so that $\hat{\mathbf{i}}_1\cdot\mathbf{S}_K^T\mathbf{S}_K\,\hat{\mathbf{i}}_1 = \mathbf{R}\hat{\mathbf{i}}_1\cdot\mathbf{S}_1^T\mathbf{S}_1\,\mathbf{R}\hat{\mathbf{i}}_1$. Observe that $\mathbf{R}\hat{\mathbf{i}}_1 = \pm\,\hat{\mathbf{i}}_1\ \forall\ \mathbf{R} \in \mathcal{P}_a$ so that $\hat{\mathbf{i}}_1\cdot\mathbf{S}_K^T\mathbf{S}_K\,\hat{\mathbf{i}}_1 = \hat{\mathbf{i}}_1\cdot\mathbf{S}_1^T\mathbf{S}_1\,\hat{\mathbf{i}}_1 = E_{11}$ for all K = 1, ..,ν. Hence, $1 \leq E_{11}$.

Now, for any tensor $\mathbf{F}$ with $\det\mathbf{F} > 0$, $\operatorname{cof}\mathbf{F} = (\det\mathbf{F})\,\mathbf{F}^{-1}$. Therefore, using the fact that $\det\mathbf{S}_1 = 1$, we can write the transpose of (2.18)(ii) as

$$\mathbf{1} = \int_{\mathcal{M}} \mathbf{A}^{-T}\, d\mu(\mathbf{A})$$

As before, operating on $\mathbf{e}$ and using Jensen's inequality, we get

$$|\mathbf{e}|^2 = \left| \int_{\mathcal{M}} \mathbf{A}^{-T}\,\mathbf{e}\, d\mu(\mathbf{A}) \right|^2 \leq \int_{\mathcal{M}} |\mathbf{A}^{-T}\,\mathbf{e}|^2\, d\mu(\mathbf{A}) \leq \max_{K=1,..,\nu} \mathbf{e}\cdot(\mathbf{S}_K^T\mathbf{S}_K)^{-1}\,\mathbf{e}.$$

As before, set $\mathbf{e} = \hat{\mathbf{i}}_1$ and observe that $\hat{\mathbf{i}}_1\cdot(\mathbf{S}_K^T\mathbf{S}_K)^{-1}\,\hat{\mathbf{i}}_1 = \hat{\mathbf{i}}_1\cdot(\mathbf{S}_1^T\mathbf{S}_1)^{-1}\hat{\mathbf{i}}_1 = (\mathbf{E}^{-1})_{11} = \dfrac{E_{22}E_{33} - E_{23}^2}{\det\mathbf{E}}$ for all K. Therefore,

$$1 \leq \frac{E_{22}E_{33} - E_{23}^2}{\det\mathbf{E}} = E_{22}E_{33} - E_{23}^2, \qquad \text{since } \det\mathbf{E} = 1.$$

Sufficiency. Assuming that (3.6) holds, we show that **1** is achieved.

Step 1: In this step, we show that Diag[1,α,γ] where $\alpha \leq \gamma$ satisfies $\alpha\gamma = 1$ is achieved.

Start with $\mathbf{F}_o = \mathbf{S}_1$. Since $\mathbf{R} = \mathbf{R}[180,\hat{\mathbf{i}}_1] \in \mathcal{P}_a$, by Remark 3.3, for a suitable $\mathbf{Q} \in SO(3)$, $\mathbf{F}_\lambda = \lambda\mathbf{Q}\mathbf{R}\mathbf{F}_o\mathbf{R} + (1-\lambda)\mathbf{F}_o$ is achieved for every $\lambda \in [0,1]$. Let $\mathbf{C}_\lambda = \mathbf{F}_\lambda^T\mathbf{F}_\lambda$. Using (3.2) and (2.12)(i) and the diagonalization procedure (Remark 3.4),

$$\mathbf{C}_o = \mathbf{S}_1^T\mathbf{S}_1 = \mathbf{E} \qquad \text{and} \qquad \mathbf{C}_{1/2} = \begin{bmatrix} \alpha^2 & 0 & 0 \\ 0 & E_{22} & E_{23} \\ 0 & E_{23} & E_{33} \end{bmatrix}.$$

Using $\det \mathbf{C}_{1/2} = (\det \mathbf{F}_{1/2})^2 = (\det \mathbf{S}_1)^2 = 1, \qquad \alpha^2 = \dfrac{1}{E_{22}E_{33} - E_{23}^2}$.

Therefore, $(\mathbf{C}_o)_{11} = E_{11}$ and $(\mathbf{C}_{1/2})_{11} = \dfrac{1}{E_{22}E_{33} - E_{23}^2}$.

By (3.6)(ii), $\dfrac{1}{E_{22}E_{33} - E_{23}^2} \le 1 \le E_{11}$. Therefore, noting that $(\mathbf{C}_\lambda)_{11}$ is a continuous function of λ, it is possible to choose $\lambda \in [0, \frac{1}{2}]$ such that $(\mathbf{C}_\lambda)_{11} = 1$. Thus we achieve $\mathbf{F}_\lambda$ such that

$$\mathbf{F}_\lambda^T\mathbf{F}_\lambda = \begin{bmatrix} 1 & \zeta & \xi \\ \zeta & E_{22} & E_{23} \\ \xi & E_{23} & E_{33} \end{bmatrix} \qquad \text{where } \zeta \text{ and } \xi \text{ depend on } \lambda.$$

Now use diagonalization first about $\hat{\mathbf{i}}_2$ and then about $\hat{\mathbf{i}}_3$ to achieve $\mathbf{F}$ such that $\mathbf{F}^T\mathbf{F} = \text{Diag}[1,\alpha^2,\gamma^2]$. Since $\det \mathbf{F}^T\mathbf{F} = (\det \mathbf{S}_1)^2 = 1$, $\alpha^2\gamma^2 = 1$. As in the case of cubic austenite, $\mathbf{R}[180,\hat{\mathbf{i}}_2 \pm \hat{\mathbf{i}}_3] \in \mathcal{P}_a$ and we can interchange the position of α and γ in $\mathbf{F}^T\mathbf{F}$ if necessary. Appealing to Remark 3.2, we achieve $\mathbf{U} = \text{Diag}[1,\alpha,\gamma]$ where $\alpha\gamma = 1$ and $\alpha \le \gamma$.

Step 2: Given that $\mathbf{U} = \text{Diag}[1,\alpha,\gamma]$, where $\alpha \le \gamma$ satisfy $\alpha\gamma = 1$, is achieved, we show in this step that $\mathbf{1}$ is achieved. This is identical to the Step 2 of the case of cubic austenite. The only case to consider is $\alpha < 1 < \gamma$. Now, $\mathbf{R} = \mathbf{R}[180,\hat{\mathbf{i}}_2+\hat{\mathbf{i}}_3] \in \mathcal{P}_a$. By Remark 3.3, for a suitable $\mathbf{Q}$, $\mathbf{F}_\lambda = \lambda\mathbf{QRUR} + (1-\lambda)\mathbf{U}$ is achieved for any $\lambda \in [0,1]$. We can calculate $\mathbf{F}_\lambda^T\mathbf{F}_\lambda$ using (3.2) and (2.12)(i). Use diagonalization about $\hat{\mathbf{i}}_2$ on $\mathbf{F}_\lambda$ to achieve $\mathbf{G}_\lambda$ such that

$$\mathbf{G}_\lambda^T\mathbf{G}_\lambda = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \beta(\lambda) & 0 \\ 0 & 0 & \alpha^2\zeta^2 + \gamma^2(1+\zeta)^2 \end{bmatrix} \qquad \text{where } \zeta = \lambda\frac{\alpha^2 - \gamma^2}{\alpha^2 + \gamma^2}.$$

By picking $\lambda = \dfrac{\gamma^2 - \sqrt{\alpha^2 + \gamma^2 - \alpha^2\gamma^2}}{\gamma^2 - \alpha^2}$, we have $\alpha^2\zeta^2 + \gamma^2(1+\zeta)^2 = 1$. As before, it is verified that $\lambda \in (0,1)$. Finally, using $\det \mathbf{G}_\lambda^T\mathbf{G}_\lambda = 1$, we see that $\beta(\lambda) = 1$. Therefore $\mathbf{G}_\lambda^T\mathbf{G}_\lambda = \mathbf{1}$ and appealing to Remark 3.2, we achieve $\mathbf{1}$.

3.3. Self-accommodation with Orthorhombic Austenite. Suppose the austenite has orthorhombic symmetry. The point group of the austenite, $\mathcal{P}_a$, is the orthorhombic group which consists of the identity and 180° rotations about three mutually perpendicular axes. The three axes $\{\hat{\mathbf{i}}_1,\hat{\mathbf{i}}_2,\hat{\mathbf{i}}_3\}$ form an orthonormal basis. All calculations are performed in this basis. There is no assumption on the symmetry of the martensite except that $\mathcal{P}_m \subset \mathcal{P}_a$ and $\mathbf{S}_1$ is any tensor with positive determinant.

Let $\mathbf{E} = \mathbf{S}_1^T\mathbf{S}_1$ and E_{ij} be the components of $\mathbf{E}$ in the orthonormal basis $\{\hat{\mathbf{i}}_1,\hat{\mathbf{i}}_2,\hat{\mathbf{i}}_3\}$. Then, the material is self-accommodating if and only if the following are true.

$$\begin{aligned}
&\text{(i)} \quad \det \mathbf{S}_1 = 1, \\
&\text{(ii)} \quad \frac{1}{E_{22}E_{33} - E_{23}^2} \le 1 \le E_{11}, \\
&\text{(iii)} \quad \frac{1}{E_{11}E_{33} - E_{13}^2} \le 1 \le E_{22} \quad \text{and} \\
&\text{(iv)} \quad \frac{1}{E_{11}E_{22} - E_{12}^2} \le 1 \le E_{33}.
\end{aligned} \tag{3.7}$$

Necessity. The necessity of the conditions (3.7) follows from the minors relation for homogeneous boundary condition and the Jensen's inequality. The proof is similar to the case of the tetragonal austenite and hence, omitted.

Sufficiency. In order to see the sufficiency, suppose $\mathbf{S}_1$ satisfies (3.7). Defining

$$\begin{aligned}
\alpha_{min}^2 &\stackrel{def}{=} \frac{1}{E_{22}E_{33} - E_{23}^2}, & \alpha_{max}^2 &\stackrel{def}{=} E_{11}, \\
\beta_{min}^2 &\stackrel{def}{=} \frac{1}{E_{11}E_{33} - E_{13}^2}, & \beta_{max}^2 &\stackrel{def}{=} E_{22}, \\
\gamma_{min}^2 &\stackrel{def}{=} \frac{1}{E_{11}E_{22} - E_{12}^2} \quad \text{and} & \gamma_{max}^2 &\stackrel{def}{=} E_{33},
\end{aligned}$$

we may rewrite (3.7) as

$$\begin{aligned}
&\text{(i)} \quad \det \mathbf{S}_1 = 1 \quad \text{and} \\
&\text{(ii)} \quad \{1,1,1\} \in [\alpha_{min}, \alpha_{max}]\times[\beta_{min}, \beta_{max}]\times[\gamma_{min}, \gamma_{max}]
\end{aligned} \tag{3.8}$$

Consider the positive numbers of α, β and γ such that

$$\alpha\beta\gamma = 1 \tag{3.9}$$

$$\{\alpha,\beta,\gamma\} \in [\alpha_{min}, \alpha_{max}]\times[\beta_{min}, \beta_{max}]\times[\gamma_{min}, \gamma_{max}]$$

In the α-β-γ space, the points $\{\alpha,\beta,\gamma\}$ satisfying (3.9) lie on the shaded surface shown in Figure 3.1. We will show that it is possible to achieve Diag[α, β, γ] for each α, β, γ satisfying (3.9). According to (3.8), {1,1,1} satisfies (3.9) and hence, **1** is achieved.

Step 1: Fix $\alpha \in [\alpha_{min}, \alpha_{max}]$.

Suppose $\mathbf{F}_o = \text{Diag}[\alpha, \beta_1, \gamma_1]$ and $\mathbf{F}_1 = \text{Diag}[\alpha, \beta_2, \gamma_2]$, $\beta_1 < \beta_2$

are achieved. By Remark 3.1, $\beta_1\gamma_1 = \beta_2\gamma_2$. Therefore, $\frac{\gamma_2}{\gamma_1} < 1 < \frac{\beta_2}{\beta_1}$ and the eigenvalues of

$$\mathbf{F}_o^{-T}\,\mathbf{F}_1^{T}\,\mathbf{F}_1\,\mathbf{F}_o^{-1} = \text{Diag}\left[\ 1,\ \left(\frac{\beta_2}{\beta_1}\right)^2,\ \left(\frac{\gamma_2}{\gamma_1}\right)^2\ \right]$$

satisfy the necessary and sufficient conditions for solving the equation $\mathbf{QF}_1 - \mathbf{F}_o = \mathbf{a} \otimes \hat{\mathbf{n}}$ for $\mathbf{Q}$, $\mathbf{a}$ and $\hat{\mathbf{n}}$ as stated in Proposition 2.1. By Remarks 3.2 and 3.3, we achieve $\mathbf{F}_\lambda = \lambda\mathbf{QF}_1 + (1-\lambda)\mathbf{F}_o$ for any $\lambda \in [0,1]$. Substituting $\lambda_1 = \left(\frac{\gamma_2}{\gamma_1}\right)^2$, $\lambda_3 = \left(\frac{\beta_2}{\beta_1}\right)^2$, $\hat{\mathbf{e}}_1 = \hat{\mathbf{i}}_3$ and $\hat{\mathbf{e}}_3 = \hat{\mathbf{i}}_2$ in (2.10), we obtain $\mathbf{a}$ and $\hat{\mathbf{n}}$. Noting that $\mathbf{F}_o^T\,\mathbf{a} \cdot \hat{\mathbf{i}}_1 = \hat{\mathbf{n}} \cdot \hat{\mathbf{i}}_1 = 0$, we can conclude from (3.2) that

$$(\mathbf{F}_\lambda^T\mathbf{F}_\lambda)_{1j} = (\mathbf{F}_o^T\mathbf{F}_o)_{1j} \qquad j = 1, 2, 3.$$

Therefore, $\mathbf{F}_\lambda^T\mathbf{F}_\lambda = \begin{bmatrix} \alpha^2 & 0 & 0 \\ 0 & \beta^2(\lambda) & \xi(\lambda) \\ 0 & \xi(\lambda) & \zeta(\lambda) \end{bmatrix}$ where β, ξ and ζ depend continuously on λ. Since $\beta^2(0) = (\mathbf{F}_o^T\mathbf{F}_o)_{22} = \beta_1^2$ and $\beta^2(1) = (\mathbf{F}_1^T\mathbf{F}_1)_{22} = \beta_2^2$, $\beta(\lambda)$ can take any value in $[\beta_1,\beta_2]$ for a suitable choice of $\lambda \in [0,1]$. Now use diagonalization about $\hat{\mathbf{i}}_3$ to achieve $\mathbf{G}_\lambda$ such that $\mathbf{G}_\lambda^T\mathbf{G}_\lambda = \text{Diag}[\alpha^2, \beta^2(\lambda), \gamma^2(\lambda)]$. Thus, appealing to Remark 3.2, it is possible to achieve Diag[α, β, γ] for each value of (β,γ) that lies on the hyperbola $\beta\gamma = \frac{1}{\alpha}$ between the points (β_1,γ_1) and (β_2,γ_2).

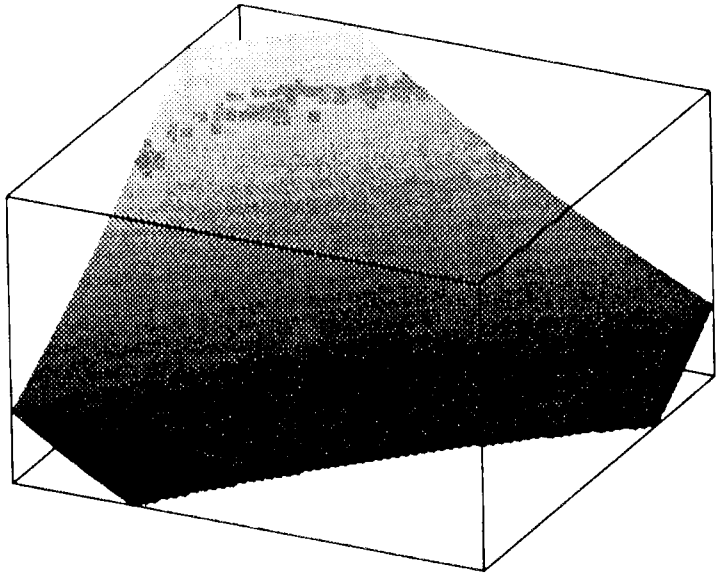

Figure 3.1: The part of the surface $\alpha\beta\gamma = 1$ within the box $[\alpha_{min},\alpha_{max}]\times[\beta_{min},\beta_{max}]\times[\gamma_{min},\gamma_{max}]$

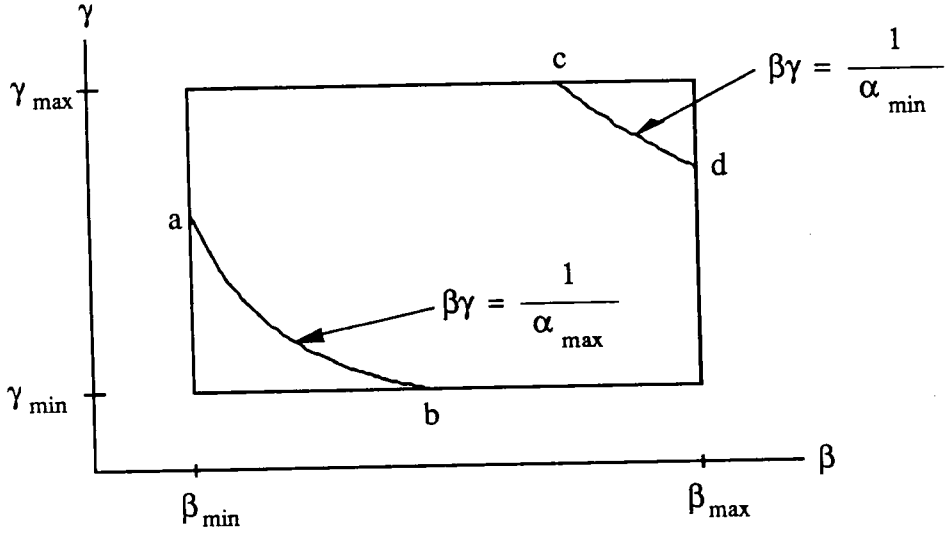

Figure 3.2: The sections of the surface $\alpha\beta\gamma = 1$ taken through the planes $\alpha = \alpha_{min}$ and $\alpha = \alpha_{max}$.

In order to complete the proof, it remains to be shown that it is possible to achieve the tensors on the boundary of the box in Figure 3.1. This is shown in Step 2.

Step 2: Let us examine the plane $\alpha = \alpha_{max}$.

Start with S_1. Use diagonalization about $\hat{i}_2$ to achieve $\mathbf{F}$ where

$$\mathbf{F}^T\mathbf{F} = \begin{bmatrix} E_{11} & 0 & E_{13} \\ 0 & \beta_{min}^2 & 0 \\ E_{13} & 0 & E_{33} \end{bmatrix} = \begin{bmatrix} \alpha_{max}^2 & 0 & E_{13} \\ 0 & \beta_{min}^2 & 0 \\ E_{13} & 0 & E_{33} \end{bmatrix}.$$

Now use diagonalization about $\hat{i}_3$ to achieve $\mathbf{G}$ where $\mathbf{G}^T\mathbf{G} = \text{Diag}\left[\alpha_{max}^2, \beta_{min}^2, \frac{1}{\alpha_{max}^2\beta_{min}^2}\right]$. By Remark 3.2, we achieve $\text{Diag}\left[\alpha_{max}, \beta_{min}, \frac{1}{\alpha_{max}\beta_{min}}\right]$ which corresponds the point (a) in Figure 3.2.

Starting with S_1, use diagonalization about $\hat{i}_3$ and then about $\hat{i}_2$ to achieve $\mathbf{F}$ where $\mathbf{F}^T\mathbf{F} = \text{Diag}\left[\alpha_{max}^2, \frac{1}{\alpha_{max}^2\gamma_{min}^2}, \gamma_{min}^2\right]$. By Remark 3.2, we achieve $\text{Diag}\left[\alpha_{max}, \frac{1}{\alpha_{max}\gamma_{min}}, \gamma_{min}\right]$ which corresponds the point (b) in Figure 3.2. Finally, by Step 1, all points in between (a) and (b) are achieved. The planes $\beta = \beta_{max}$ and $\gamma = \gamma_{max}$ are treated similarly.

Let us now examine the plane $\alpha = \alpha_{min}$.

Starting with S_1, use diagonalization first about $\hat{i}_1$ and then about $\hat{i}_2$ to achieve $\mathbf{F}$ where $\mathbf{F}^T\mathbf{F} = \text{Diag}\left[\alpha_{min}^2, \frac{1}{\alpha_{min}^2\gamma_{max}^2}, \gamma_{max}^2\right]$. By Remark 3.2, we achieve $\text{Diag}\left[\alpha_{min}, \frac{1}{\alpha_{min}\gamma_{max}}, \gamma_{max}\right]$ which corresponds the point (c) in Figure 3.2. Starting with S_1, use diagonalization first about $\hat{i}_1$ and then about $\hat{i}_3$ to achieve $\mathbf{F}$ where $\mathbf{F}^T\mathbf{F} = \text{Diag}\left[\alpha_{min}^2, \beta_{max}^2, \frac{1}{\alpha_{min}^2\beta_{max}^2}\right]$. By Remark 3.2, we achieve $\text{Diag}\left[\alpha_{min}, \beta_{max}, \frac{1}{\alpha_{min}\beta_{max}}\right]$ which corresponds the point (d) in Figure 3.2. Finally all points in between (c) and (d) are achieved by step 1. The planes $\beta = \beta_{min}$ and $\gamma = \gamma_{min}$ are treated similarly.

3.4. Self-accommodation with Monoclinic Austenite. Suppose the symmetry of the austenite is monoclinic. $\mathcal{P}_a$ consists of the identity and $\mathbf{R} = \mathbf{R}[180,\hat{\mathbf{i}}]$ for some $\hat{\mathbf{i}}$. The only crystallographic subgroup of the monoclinic group is the triclinic group, which contains only one element, the identity. Thus, in this case we need to consider only the monoclinic to the triclinic transition. According to (2.3), there are two variants of martensite with variants $\mathbf{S}_1$ and $\mathbf{S}_2$ which satisfy $\mathbf{RS}_1\mathbf{R} = \mathbf{S}_2$. Therefore from Remark 2.1,

(i) $\mathbf{QS}_2 - \mathbf{S}_1 = \mathbf{a} \otimes \hat{\mathbf{n}}$ for some vectors $\mathbf{a}$ and $\hat{\mathbf{n}}$ and some $\mathbf{Q} \in SO(3)$ and (3.10)

(ii) $\det \mathbf{S}_1 = \det \mathbf{S}_2$.

In this case, Ball and James[10] have characterized all microstructures whose Young measure supported is on $\mathcal{M}$. We adopt their result.

Let $\mathbf{Q}$, $\mathbf{a}$, and $\hat{\mathbf{n}}$ solve $\mathbf{QS}_2 - \mathbf{S}_1 = \mathbf{a} \otimes \hat{\mathbf{n}}$ (for example according to (2.12)(ii)).

Define $\delta \stackrel{\text{def}}{=} \frac{1}{2} |\mathbf{a}|\,|\mathbf{S}_1^{-T}\hat{\mathbf{n}}|$, $\hat{\mathbf{e}}_3 \stackrel{\text{def}}{=} \dfrac{\mathbf{a}}{|\mathbf{a}|}$, $\hat{\mathbf{e}}_1 \stackrel{\text{def}}{=} \dfrac{\mathbf{S}_1^{-T}\hat{\mathbf{n}}}{|\mathbf{S}_1^{-T}\hat{\mathbf{n}}|}$

$$\mathbf{L} \stackrel{\text{def}}{=} \mathbf{S}_1^{-1}(\mathbf{1} - \delta\,\hat{\mathbf{e}}_3 \otimes \hat{\mathbf{e}}_1) \quad \text{and} \quad (3.11)$$

$$\mathbf{D} \stackrel{\text{def}}{=} \mathbf{L}^T\mathbf{L}.$$

Then, in order for a material to form a self-accommodating microstructure, it is necessary and sufficient that in the orthonormal basis $\{\hat{\mathbf{e}}_1,\hat{\mathbf{e}}_2,\hat{\mathbf{e}}_3\}$,

$$\mathbf{D} = \begin{bmatrix} D_{11} & 0 & D_{13} \\ 0 & 1 & 0 \\ D_{13} & 0 & D_{33} \end{bmatrix} \quad \text{where} \quad (3.12)$$

$$0 < D_{11} < 1 + \delta^2, \quad 0 < D_{33} < 1 \quad \text{and} \quad D_{11}D_{33} - D_{13}^2 = 1.$$

This follows immediately from Ball and James[10] who show that a sequence $\mathbf{y}^k \overset{*}{\rightharpoonup} \mathbf{y}$ in $W^{1,\infty}(\Omega\,;\,\mathbb{R}^3)$ satisfies supp $\nu_{\mathbf{x}} \subset \mathcal{M}$, a.e $\mathbf{x} \in \Omega$ if and only if $\mathbf{D}(\mathbf{x}) = \mathbf{L}^T(\nabla\mathbf{y}(\mathbf{x}))^T\nabla\mathbf{y}(\mathbf{x})\,\mathbf{L}$ satisfies (3.12) a.e. $\mathbf{x} \in \Omega$.

Remark 3.5. Suppose $\det \mathbf{S}_1 \neq 1$. We ask the question whether the material can form a microstructure which is a pure dilatation with respect to the austenite, i.e., is it possible to ahieve $\alpha\mathbf{1}$ where $\alpha = (\det \mathbf{S}_1)^{1/3}$? By scaling, ($\mathbf{y}^k \longmapsto \frac{1}{\alpha}\mathbf{y}^k$) it is clear that this is true if and only if a material with transformation strain $\frac{1}{\alpha}\mathbf{S}_1$ is self-accommodating. Since $\det(\frac{1}{\alpha}\mathbf{S}_1) = 1$, this is always true in the case of cubic austenite. However, the answer is not true in general for the other cases because the restrictions on $\mathbf{E}$ listed in Table 3.1 are not invariant under this scaling. □

§4. COMPARISON OF THEORY WITH EXPERIMENT

In order to make any comparison of theory and experiment, it is necessary to calculate the transformation strain from the lattice parameters of both the austenite and the martensite measured at the transformation temperature. Unfortunately, such measurements were not always found in the literature. Often, all that was found were parameters for the austenite measured by one researcher at some temperature and those for the martensite measured by a different researcher at a different temperature. Similarly, the shape-memory effect was observed by one researcher while the lattice parameters were measured by others. Furthermore, in some cases the parameters had to be read off from graphs plotted on rather coarse scales. Strictly speaking, the relations derived in Section 3 are true only at the transformation temperature. As we go away form this temperature, thermal expansion changes the lattice parameters. Similarly, the lattice parameters change with composition, which unavoidably differs in specimens used by the different researchers. We shall keep these in mind while making any comparison.

Table 4.1 shows the percentage change in volume during transformation of various alloys with cubic austenite. Also see Figure 5.2 for the lattice parameters of some alloys undergoing the cubic to tetragonal transformation. The common, well-known shape-memory alloys like Ni-Ti, Cu-Al-Ni, Ni-Al, Cu-Al and Cu-Zn-Al have small transformation volume change. Moreover, the volume seems to decrease in these alloys during the transformation from austenite to martensite. Often, the lattice parameters of the austenite are measured at a high temperature while those of the martensite are measured at a low temperature. Therefore, part of the decrease in volume can be attributed to thermal expansion across this temperature difference. Ferrous steels have larger volume changes. Moreover, the volume increases during the transformation from the austenite to the martensite. Zirconia undergoes a tetragonal to monoclinic transformation accompanied by a volume change of approximately 3%[61]. This transformation often results in the cracking of the specimen.

The observations of Arlt[3] in polycrystals of $BaTiO_3$ and $YBa_2Cu_3O_{7-\delta}$ are very interesting. $BaTiO_3$ undergoes a volume preserving cubic to tetragonal transformation[33]. $YBa_2Cu_3O_{7-\delta}$ undergoes a first order tetragonal to orthorhombic transformation which may be induced either by temperature or by diffusion of oxygen. Arlt takes aged polycrystals which have completely transformed from the high to the low symmetry phase. He carefully cuts out a slice in order to reveal the microstructure deep in the interior of the polycrystal. He studies the microstructure using both optical and electron microscope. The grains of $BaTiO_3$ show no cracks

Table 4.1: The measured transformation volume change in some alloys with cubic austenite

Alloy	Symmetry of Martensite	Percentage Volume change $100(1 - \det S_1)$	Shape-mem.?	Comments and Ref.
Ni-36% Al	Tetragonal	0.305	Yes	17,21
Ni -49.4% Mn	Tetragonal	0.725	?	1,41
Ni-48% Zn-20% Cu	Tetragonal	0.820	Yes	Lattice parameters were read off a graph [48,49]
Ni-34% Zn-15% Si	Tetragonal	- 0.139	Yes	Lattice parameters were read off a graph [48]
In-22.73% Tl	Tetragonal	0.046	Yes	35,53
Fe-31.2% Pd	Tetragonal	0.2	Yes	60
Fe-24% Pt	Tetragonal	- 0.0	Yes	62
Fe-31% Ni-0.3% C	Tetragonal	- 1.833	No	54
Fe-7.9% Cr-1.1% C	Tetragonal	- 2.568	No	47
Fe-7% Al-2% C	Tetragonal	-2.414	No	68
Cu-14.2 wt.% Al -4.3 wt.% Ni	Orthorhombic	0.297	Yes	55
Au-47.5% Cd	Orthorhombic	0.413	Yes	14,18
Ag-52 wt.% Cd	Orthorhombic	0.157	Yes	44
Zr-19.5% Th	Orthorhombic	2.22	No	36
Ni-50% Ti	Monoclinic	0.023	Yes	Most commonly used shape-memory alloy.[42,46]
Cu-17.2% Al -13.3%Zn	Monoclinic (18R)	0.356	Yes	58
Cu - Zn - Ga	Monoclinic (18R)	1.06	Yes	58
Cu - Al	Monoclinic (18R)	"approx. zero"	Yes	65
All compositions are in at. % at unless indicated otherwise. The temperature is given in °C.				

and there is no mismatch at the boundaries suggesting self-accommodation. In contrast, there is significant cracking and grain boundary mismatch in $YBa_2Cu_3O_{7-\delta}$. In a tetragonal to orthorhombic transformation, $S_1 = Diag[\alpha,\beta,\gamma]$ in an orthonormal basis parallel to the edges of the tetragonal unit cell. If $\hat{i}_1$ is the c-axis of the tetragonal unit cell, according to Table 3.1, $\alpha = \beta\gamma = 1$ is necessary and sufficient for self-accommodation. The measured value[2] of $S_1 = Diag[0.9887,0.9898,1.0068]$ for $YBa_2Cu_3O_{7-\delta}$ clearly does not satisfy that condition. Arlt also remarks that the cracks lie in a plane perpendicular to $\hat{i}_1$ indicating that they arise as a result of the lack of accommodation in the direction of the c-axis. These remarks should be tempered with the observation due to Van Tendeloo[67] that cracking in $YBa_2Cu_3O_{7-\delta}$ is a result of the creation of Oxygen-rich atomic layers by diffusion in the presence of moisture.

In summary, in cases where comparisons are possible, the overall agreement between the experiments and the predictions of Table 3.1 are quite satisfactory.

§5. CONCLUSIONS AND DISCUSSION

Self-accommodation is an inherent feature of the one-way shape-memory effect. It may also be important for the reversibility of transformation in polycrystals and for the easy nucleation of martensite during cooling. The main result of the paper is summarized in Table 3.1. It lists necessary and sufficient conditions that the transformation strain of a material has to satisfy in order to be able to form a self-accommodating microstructure. Materials whose austenite phase is cubic are self-accommodating if and only if the transformation is volume preserving. If the symmetry of the austenite is not cubic, the material has to satisfy additional, rather strict conditions in order to be self-accommodating. These results agree quite well with the experimental observations in cases where comparisons are possible.

The analysis in this paper, however, does not include any mechanism for the nucleation and growth of martensite into the austenite during cooling. In coarse grained specimens of shape-memory alloys, a wedge-like or spear-like microstructure schematically shown in Figure 5.1 is often seen. During cooling, wedge-shaped domains of martensite grow into the austenite[55,63]. This microstructure provides an easy way for the initiation of transformation[55] and is thus important for thermoelasticity and reversibility of transformation. Bhattacharya[12] found that such a microstructure is coherent if and only if the lattice parameters of the material satisfy certain conditions. For example, in a cubic to tetragonal transformation, there are three variants of martensite defined by

$$\mathbf{S}_i = \eta_1 \mathbf{1} + (\eta_2 - \eta_1)\, \hat{\mathbf{i}}_i \otimes \hat{\mathbf{i}}_i \qquad i = 1, 2, 3, \tag{5.1}$$

where $\{\hat{\mathbf{i}}_1, \hat{\mathbf{i}}_2, \hat{\mathbf{i}}_3\}$ is an orthonormal basis parallel to the edges of the cubic unit cell. Here, η_1 and η_2 are positive constants determined by the lattice parameters of both the austenite and the martensite lattice. For example, in Ni-Al $\eta_1 = 0.9392$ and $\eta_2 = 1.1302$[17]. Coherence of the wedge-like microstructure forces η_1 and η_2 to satisfy[12]

$$\eta_1^2 = \frac{(1 - \eta_2^2)^2 + 4\,\eta_2^2\,(1 + \eta_2^2)}{(1 - \eta_2^2)^2 + 8\,\eta_2^4}.$$

Figure 5.2 shows plots of this relation as well as the relation $\eta_1^2 \eta_2 = 1$ (which corresponds to volume preserving transformation) in the η_1 - η_2 plane. It is interesting to observe that these two curves are very close to each other when (η_1, η_2) is close to (1,1), the values of practical interest.

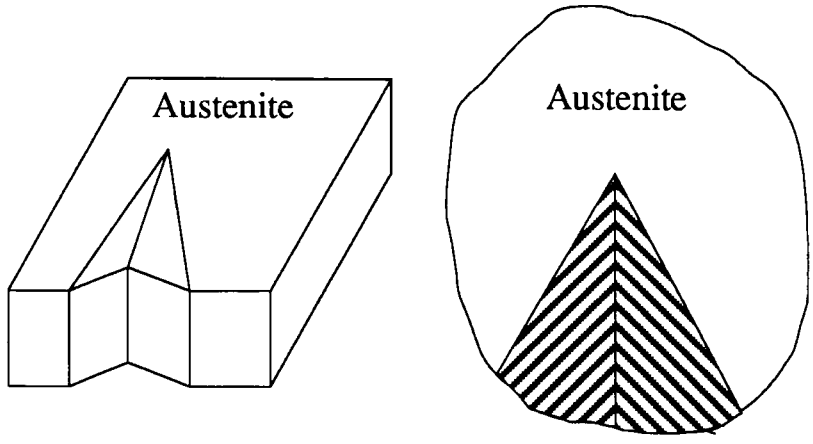

Figure 5.1: The schematic view of a wedge-like deformation. The figure on the left shows the wedge in a three dimensional specimen and the one on the right shows a typical cross-section.

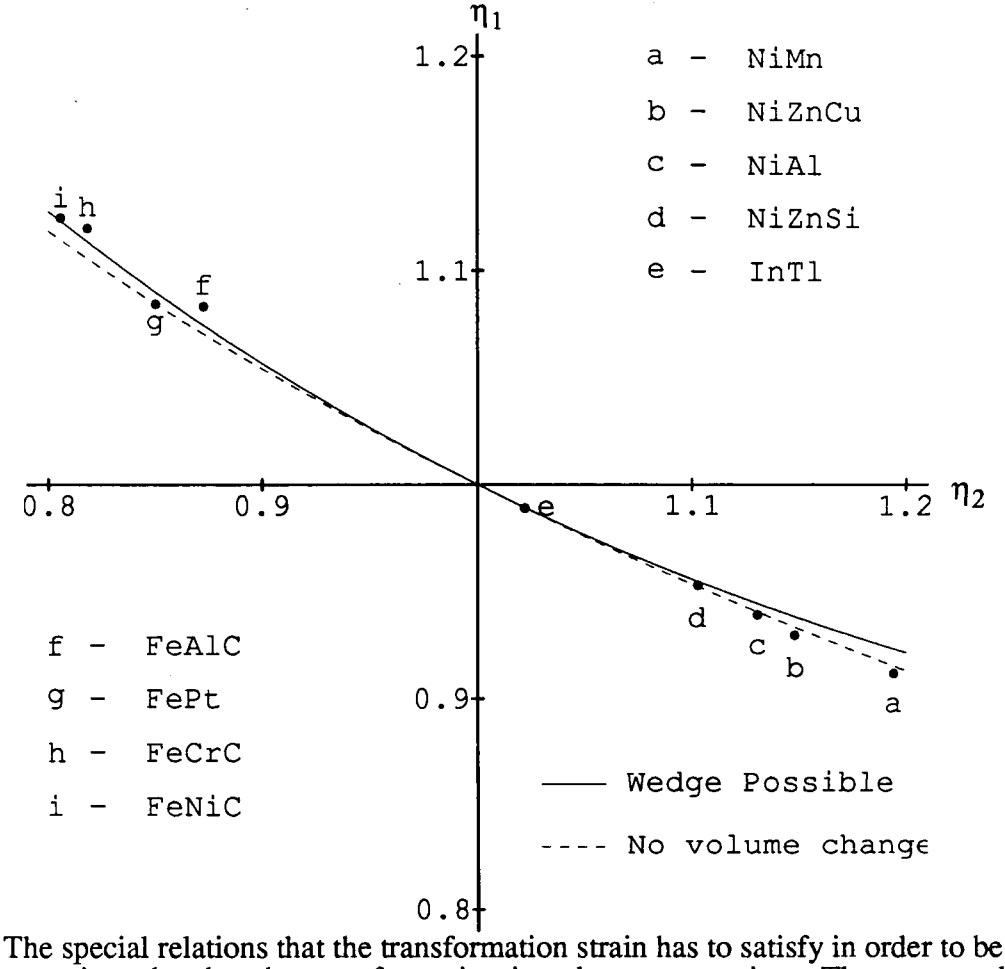

Figure 5.2: The special relations that the transformation strain has to satisfy in order to be able to form a wedge or in order that the transformation is volume preserving. The measured lattice parameters of some common alloys are also plotted. Refer to Table 4.1 for details about the alloys.

Similarly, in the case of the cubic to orthorhombic transformation, there are six variants of martensite and

$$S_1 = \begin{bmatrix} \frac{\alpha+\gamma}{2} & 0 & \frac{\alpha-\gamma}{2} \\ 0 & \beta & 0 \\ \frac{\alpha-\gamma}{2} & 0 & \frac{\alpha+\gamma}{2} \end{bmatrix}$$ in an orthonormal basis parallel to the cubic unit cell.

α, β and γ are positive constants determined by the lattice parameters of both the austenite and the martensite lattices. A material undergoing this kind of transformation can form a wedge if and if it lies on a certain family of surfaces in α-β-γ space[12]. The transformation is volume preserving if and only if the material lies on the surface $\alpha\beta\gamma = 1$. Thus, a material is self-accommodating and can form a wedge if and only if it lies on the intersection of the family of wedge-surfaces with the surface $\alpha\beta\gamma = 1$. This intersection is a family of curves in α-β-γ space whose projection on the α-γ plane is shown in solid lines in Figure 5.3. On any of these curves, $\beta = \frac{1}{\alpha\gamma}$. The reasoning in this paper suggest that good a shape-memory alloy in which wedge-like microstructures are seen should lie on one of these curves. It turns out that Cu-Al-Ni does not. However, Cu-Al-Ni lies very close to one the wedge-surfaces[12] and has very small volume change (Table 4.1). In order to understand this apparent contradiction, let us examine the intersection of one of the wedge-surfaces with the plane $\beta = 0.9178$ (which corresponds to the measured value for Cu-Al-Ni). This intersection is a curve which can be parametrized by α. Figure 5.4 is a plot of the percentage volume change ($100\ (1 - \alpha\beta\gamma)$) along this curve plotted as a function of α. Though the volume change is zero at just two points, observe that the volume change is very small for a whole range of of values of α. Thus, going back to the α-β-γ space, though the wedge-surfaces intersect the surface of zero volume change only on some curves, large portions of these wedge-surfaces lie very close to the surface of zero volume change. The shaded region in Figure 5.3 is the projection on the α-γ plane of those regions of the family of wedge-surfaces in which the transformation volume change is less that 0.5%. Therefore, if the measured values of (α,γ) for a given material which undergoes small change in volume during transformation lies in the shaded region, the material lies close to one amongst the family of the surfaces on which it is possible to form a wedge.

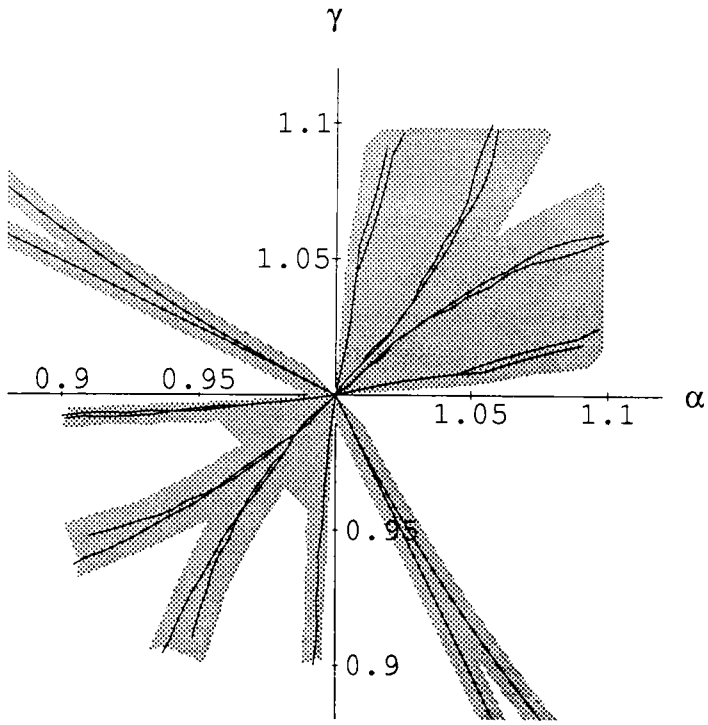

Figure 5.3: Projection of the curves on which it is possible to form both a wedge-like and a self-accommodating microstructure. The shaded regions are the projection of those portions of the wedge surfaces where the volume change is less than 0.5%

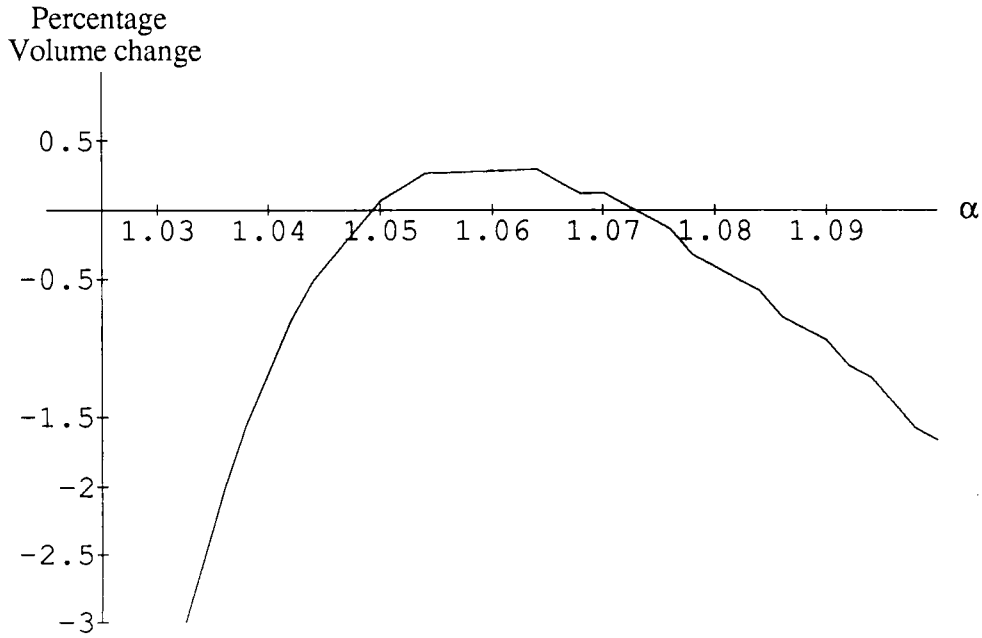

Figure 5.4: Percentage volume change (100(1 - det $\mathbf{S}_1$)) along the curve of intersection of one amongst the family of wedge surface with the plane $\beta = 0.9178$.

The lucky accident that these two relations are close to each other suggests that a self-accommodating material with cubic austenite can form the wedge-like microstructure with small elastic energy. Therefore, it is an ideal candidate for displaying the shape-memory effect. On the other hand materials which do not have cubic austenite have to satisfy very strict relations in order to be self-accommodating. Thus, it is a reasonable to conclude that shape-memory materials must have cubic austenite and must undergo a volume preserving transformation. In fact, this is one of the empirical criteria currently being used to invent ferrous shape-memory alloys[43,45].

The self-accommodating microstructure that we constructed in Section 3 was a laminate with several levels. However, in an actual material, it is uncommon to see a laminate with more than two, at most three, levels. We speculate on the possible reasons. Firstly, the construction in Section 3 treats martensites of all symmetries alike. It so happens that it is possible to construct laminates with fewer levels in special cases. For example, in a cubic to tetragonal transformation, $\mathbf{S}_1$ given by (5.1) is already diagonal so that we may skip Step 1 in the construction described in Section 3.1. Secondly, it is common in these problems involving microstructure to have a high degree of non-uniqueness[10]. The construction in Section 3 is just one self-accommodating microstructure and there may exist many self-accommodating microstructures, especially if one also considers non-homogeneous microstructures. In actual materials, non-homogeneous microstructures are typically seen[63]. Therefore, one can speculate that there are self-accommodating microstructures which are not homogeneous and which do not involve laminates of more that two or three levels.

Finally, the following idea is very suggestive. Suppose we want to satisfy the homogeneous boundary conditions $\mathbf{F}_0\mathbf{x}$ on $\partial\Omega$. Suppose $\{\mathbf{y}^k\}$ is a laminate with n levels and has an average deformation gradient $\mathbf{F}$ where $|\mathbf{F}_0 - \mathbf{F}|$ is small. Notice that $\mathbf{y}^k$ satisfies $\mathbf{F}\mathbf{x}$ on $\partial\Omega$. Further, let the Young measure of the laminate, $\nu_{\mathbf{x}}[\{\mathbf{y}^k\}]$, be supported on $\mathcal{M}$. Now, consider the sequence $\mathbf{z}^k(\mathbf{x}) = \mathbf{F}_0\mathbf{F}^{-1}\mathbf{y}^k(\mathbf{x})$. $\{\mathbf{z}^k\}$ is also a laminate with n levels and average deformation gradient $\mathbf{F}_0$. It also satisfies the boundary condition $\mathbf{F}_0\mathbf{x}$ on $\partial\Omega$. Now, $\nabla\mathbf{z}^k(\mathbf{x}) = \mathbf{F}_0\mathbf{F}^{-1}\nabla\mathbf{y}^k(\mathbf{x})$. Since $\mathbf{F}_0\mathbf{F}^{-1}$ is close to identity, $\nabla\mathbf{z}^k(\mathbf{x})$ is close $\nabla\mathbf{y}^k(\mathbf{x})$. Therefore, the Young measure, $\nu_{\mathbf{x}}[\{\mathbf{z}^k\}]$, is supported on tensors which are close to $\mathcal{M}$. Therefore, if the free energy ϕ is smooth, $\mathcal{E}_\Omega[\mathbf{z}^k,\theta_0]$ becomes very small as $k \to \infty$. Thus, the material can satisfy the prescribed boundary conditions using a laminate with n levels which has a small energy. In the thermoelasticity theory being used here, the surface energy is neglected as are any dynamic effects and hysteresis. There is no notion of metastability either. It is possible that the laminate above is metastable in a theory that takes these into account.

The results of Ball and James[10] in the case of the two well problem can be used to derive some interesting estimates. As mentioned earlier, they study the special case when there are two variants of martensite $\mathbf{S}_1$ and $\mathbf{S}_2$ that satisfy (3.10). For definiteness, we consider the case arising out of the tetragonal to orthorhombic transformation where

$$\mathbf{S}_1 = \text{Diag}[\alpha,\beta,\gamma] \qquad \text{and} \qquad \mathbf{S}_2 = \text{Diag}[\alpha,\gamma,\beta], \qquad \beta \le \gamma$$

in an orthonormal basis $\{ \hat{\mathbf{i}}_1, \hat{\mathbf{i}}_2, \hat{\mathbf{i}}_3 \}$ parallel to the edges of the tetragonal unit cell are the two variants. We have chosen $\hat{\mathbf{i}}_1$ as the c-axis of the tetragonal lattice.

Define $$\mathcal{D}_0 \stackrel{\text{def}}{=} \left\{ \mathbf{F}_0 \mid \mathbf{F}_0 \text{ is achieved} \right\} .$$

Recall that we say that $\mathbf{F}_0$ is achieved if there is a microstructure with Young measure supported on $\mathcal{M}$ which satisfies the homogeneous boundary condition $\mathbf{F}_0\mathbf{x}$ on $\partial\Omega$. The results of Ball and James[10] can be adapted to show that $\mathbf{F}_0 \in \mathcal{D}_0$ if and only if

$$(\mathbf{F}_0^T\mathbf{F}_0)_{22} + (\mathbf{F}_0^T\mathbf{F}_0)_{33} \pm (\mathbf{F}_0^T\mathbf{F}_0)_{23} \le \beta^2 + \gamma^2 \qquad \text{and} \qquad \det \mathbf{F}_0 = \det \mathbf{S}_1.$$

Moreover, every $\mathbf{F}_0 \in \mathcal{D}_0$ can be achieved by a double laminate, though not necessarily by a single laminate. However, for every $\mathbf{F}_0 \in \mathcal{D}_0$, there is a single laminate with average deformation gradient $\mathbf{F}_1$ such that

$$| \mathbf{F}_0^T\mathbf{F}_0 - \mathbf{F}_1^T\mathbf{F}_1 | \qquad \le \qquad \frac{1}{4} \frac{(\gamma^2 - \beta^2)^4}{(\gamma^2 + \beta^2)^2} .$$

On the other hand, it is possible to find a particular $\mathbf{F}_0 \in \mathcal{D}_0$* such that

$$| \mathbf{F}_0^T\mathbf{F}_0 - \mathbf{S}_I^T\mathbf{S}_I | \qquad \ge \qquad \gamma(\gamma - \beta) \qquad\qquad I = 1,2.$$

In problems of practical interest, β and γ are both close to 1. Therefore, $|\mathbf{F}_0^T\mathbf{F}_0 - \mathbf{F}_1^T\mathbf{F}_1| = O(|\gamma - \beta|^4)$ is small and using arguments presented earlier, it is possible satisfy the boundary condition $\mathbf{F}_0\mathbf{x}$ on $\partial\Omega$ using a single laminate whose energy is very small. However, since $|\mathbf{F}_0^T\mathbf{F}_0 - \mathbf{S}_I^T\mathbf{S}_I| \ge O(|\gamma - \beta|)$, the homogeneous deformation will require relatively large energy. In fact, the pictures of polycrytalline $YBa_2Cu_3O_{7-\delta}$ by Arlt[3] shows that the microstructure is predominantly a single laminate.

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*For example, $\mathbf{F}_0 = \text{Diag}[\alpha, \sqrt{\beta\gamma}, \sqrt{\beta\gamma}]$.

Similarly, consider a volume preserving cubic to tetragonal transformation. There are three variants of martensite and $\mathbf{S}_i$ are given by (5.1) with η_1 and η_2 satisfying $\eta_1^2 \eta_2 = 1$. As we saw in Section 3, it is possible to construct a self-accommodating microstructure. How well can this be approximated by a single laminate? For any i,j $\in \{1,2,3\}$, it is possible to find $\mathbf{Q} \in SO(3)$ such that $\mathbf{QS}_i - \mathbf{S}_j = \mathbf{a} \otimes \hat{\mathbf{n}}$ if $i \neq j$[10]. Therefore, it is possible to form a single laminate with the support of the Young measure contained in $\mathcal{M}$ and with average deformation gradient $\mathbf{F}_1 = \lambda \mathbf{QS}_i + (1-\lambda)\mathbf{S}_j$ for some $\lambda \in [0,1]$. Therefore it is a matter of calculation to find that

$$\mathbf{F}_1^T\mathbf{F}_1 = \begin{bmatrix} \alpha & \delta & 0 \\ \delta & \beta & 0 \\ 0 & 0 & \eta_1^2 \end{bmatrix}$$

in the basis $\{\hat{\mathbf{i}}_j, \hat{\mathbf{i}}_i, \hat{\mathbf{i}}_j \wedge \hat{\mathbf{i}}_i\}$ where
α, β and δ are functions of λ and η_1.

Hence, for any single laminate with Young measure supported on $\mathcal{M}$, the average deformation gradient $\mathbf{F}_1$ satisfies.

$$| \mathbf{F}_1^T\mathbf{F}_1 - \mathbf{1} | \geq | \eta_1^2 - 1 | = | \frac{1}{\eta_2} - 1 |.$$

However, we can do substantially better with a double laminate whose Young measure is supported on $\mathcal{M}$. Laminate $\mathbf{S}_1$ with $\mathbf{QS}_2$ (for a suitable $\mathbf{Q}$) to obtain an average deformation gradient $\frac{2}{3}\mathbf{QS}_2 - \frac{1}{3}\mathbf{S}_1$. Let $\mathbf{R} = \mathbf{R}[180, \hat{\mathbf{i}}_2 + \hat{\mathbf{i}}_3]$. Notice that $\mathbf{R} \in \mathcal{P}_a$. Therefore, for a suitable $\mathbf{Q}_o$, there is double laminate with average deformation gradient

$$\mathbf{F}_2 = \tfrac{1}{2}\mathbf{Q}_o(\tfrac{2}{3}\mathbf{QS}_2 - \tfrac{1}{3}\mathbf{S}_1)\mathbf{R} + \tfrac{1}{2}(\tfrac{2}{3}\mathbf{QS}_2 - \tfrac{1}{3}\mathbf{S}_1).$$

In Figure 5.5, the solid curve is a plot of $| \mathbf{F}_2^T\mathbf{F}_2 - \mathbf{1} |$ as a function of η_2. The dotted line is a plot of $| \mathbf{F}_1^T\mathbf{F}_1 - \mathbf{1} | = | \frac{1}{\eta_2} - 1 |$. Thus, the best singe level laminate has an approximating error (in $| \, |$ norm) on or above the dotted line, while the best double level laminate has an approximating error on or below the solid line. Therefore, using arguments presented earlier, in a volume preserving cubic to tetragonal transformation, we can find a double laminate which likely has small energy and satisfies boundary conditions corresponding to self-accommodation. In fact, the pictures of polycrystalline $BaTiO_3$ by Arlt[3] shows a fairly homogeneous double laminate, despite some refining at the boundaries and occasional inhomogeneities.

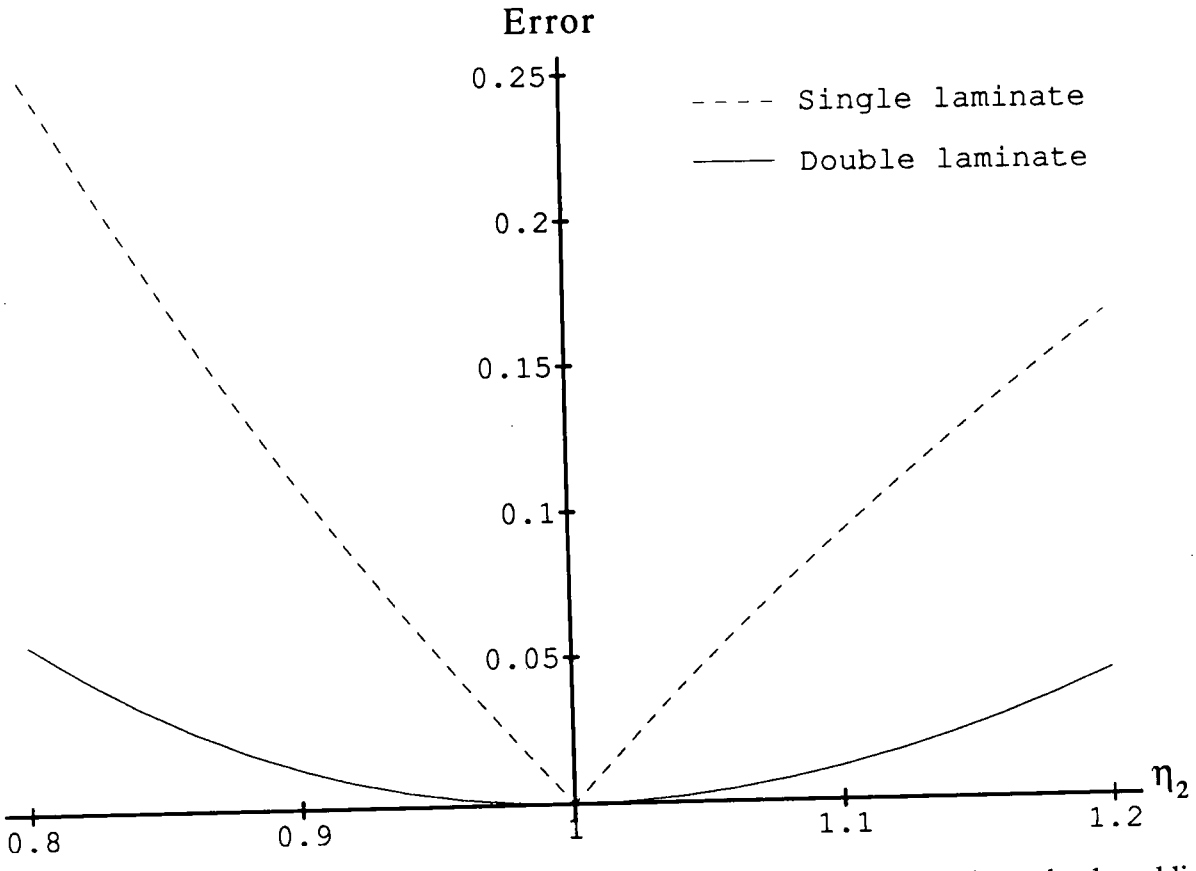


Figure 5.5: The best singe level laminate has an approximating error on or above the dotted line, while the best double level laminate has an approximating error on or below the solid line.

APPENDIX: SELF-ACCOMMODATING PLATE GROUPS

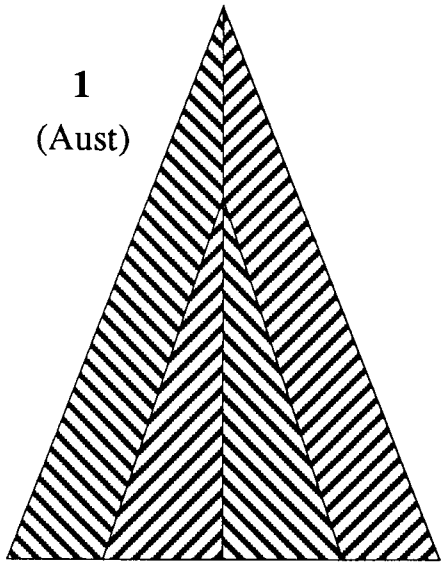
In general, only very rare materials can form a coherent interface of the austenite and a single variant of martensite. The Hadamard jump condition for such an interface requires that one of the eigenvalues of $\mathbf{S}_1$ is equal to one[9]. The only material known to me that satisfies this condition is Ti - 21at. % Ta[16]. In this alloy, Bywater and Christian varied the composition until the middle eigenvalue became equal to one. However, it is very common to find a set of fine twins (laminates) forming a coherent interface with the austenite. This follows from the fact that coherence now requires the less restrictive set of conditions[9]

$$\mathbf{Q}\mathbf{S}_I - \mathbf{S}_J = \mathbf{a} \otimes \hat{\mathbf{n}} \tag{A1}$$

$$\mathbf{Q}_o (\lambda \mathbf{Q}\mathbf{S}_I + (1-\lambda) \mathbf{S}_J) - \mathbf{1} = \mathbf{b} \otimes \hat{\mathbf{m}}$$

hold for some $I,J \in \{1, \ldots, \nu\}$, $\lambda \in (0,1)$, $\mathbf{Q}_o, \mathbf{Q} \in SO(3)$ and vectors $\mathbf{a}$, $\mathbf{b}$, $\hat{\mathbf{n}}$ and $\hat{\mathbf{m}}$. $\hat{\mathbf{n}}$ is the normal to the twin planes and $\hat{\mathbf{m}}$ is the normal to the austenite-martensite interface. It turns out that it is possible to satisfy (A1) for a vast range of values $\mathbf{S}_1$. This is the well-known crystallographic theory of martensite developed independently by Wechsler, Leiberman and Read[69] and Bowles and MacKenzie[15]. Also see Ball and James[9] and Bhattacharya[12] for a description of the set of values of $\mathbf{S}_1$ that permit the existence of an austenite-martensite interface.

In all the shape-memory alloys found in the literature, the austenite has cubic symmetry. Tas, Delaey and Deruyterre[65] and Saburi and Wayman[58] found that in a large number of shape-memory alloys, there are 24 symmetry related solutions to (A1). Moreover, in every solution, the austenite-martensite interface is close to one of the {110} family of planes in the cubic austenite i.e, in the cubic basis, $\hat{\mathbf{m}}$ is close to some permutation of the vector $\{1,\pm1,0\}$. There are six crystallographically equivalent {110} planes in a cubic lattice. Thus, one can classify the 24 possible austenite-martensite interfaces into six sets. Each set of four austenite-martensite interfaces (or equivalently, the set of four fine twins of martensite, each of which has an average deformation gradient of the form $\mathbf{1} + \mathbf{b} \otimes \hat{\mathbf{m}}$ which forms the interface) is known as a "plate group". Furthermore, in Cu-Al, Tas et. al. and in a variety of other shape-memory alloy, Saburi and Wayman found that the sum of the average deformation gradients of the four sets of fine twins that comprise each plate group is close to $4\mathbf{1}$. Therefore, they concluded, a microstructure consisting of the four sets of fine twins in a plate group arranged in four subdomains of equal volume would be self-accommodating.



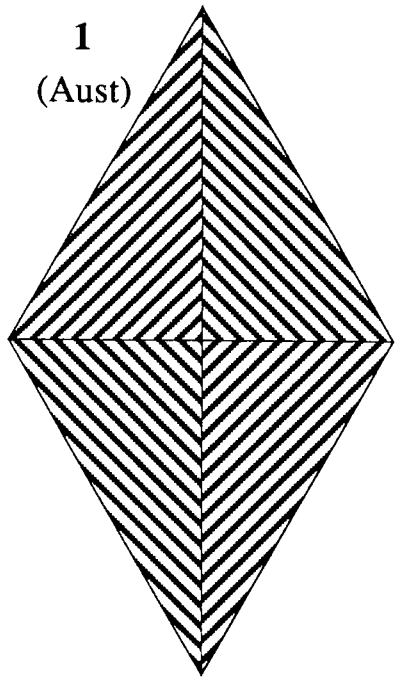


Figure A1 a

Figure A1 b

Figure A1: A schematic view of the microstructure using self-accommodating plate groups.

However, it is not clear whether they use our strict definition of self-accommodation (i.e., $y^k(x) = x$ on $\partial\Omega$). Tas et. al. suggested the microstructure shown in Figure A1a while Saburi and Wayman suggested the diamond microstructure shown in Figure A1b. Owing to its geometric simplicity, the diamond microstructure has found widespread acceptance in the metallurgical literature. Notice that it is not clear whether the microstructure Figure A1a can be surrounded by a sea of austenite on all sides. Similarly Figure A1b satisfies homogeneous boundary conditions corresponding to the austenite only in the plane; but it is not clear what happens out of plane. The self-accommodating microstructure observed by Tan and Xu[63] to a degree resembles the diamond microstructure, but clearly involves more than four sets of fine twins.

Moreover, the proposed microstructure is not coherent according to the concept of coherence being used here. One way to seeing this is by checking the jump condition at each interface as Bhattacharya[12] did for the wedge-like microstructure. Consider for example the diamond microstructure. It consists of two back to back wedges described in Section 5. Recall that the coherence condition of the wedge-like microstructure imposed certain strict restrictions on the transformation strain. It turns out that the coherence condition of putting two wedges back to

back imposes further, apparently impossible restrictions on the transformation strain. Checking individual jump conditions is a long and cumbersome procedure. Moreover, it is specific to the microstructure. Here we use a different method that demonstrates the power of the minors relations.

Suppose we have a coherent microstructure that satisfies a homogeneous boundary condition $\mathbf{y}(\mathbf{x}) = \mathbf{F}_o\mathbf{x}$ on $\partial\Omega$ using n sets of fine twins with average deformation gradients $\mathbf{1} + \mathbf{b}_i \otimes \hat{\mathbf{m}}_i$, i = 1,2, ..,n. Let $\mathbf{A}_i$ and $\mathbf{B}_i$ (that satisfy $\mathbf{B}_i - \mathbf{A}_i = \mathbf{a}_i \otimes \hat{\mathbf{n}}_i$) form fine twins in the proportion μ_i. By assumption,

$$\mu_i \mathbf{B}_i + (1-\mu_i)\mathbf{A}_i = \mathbf{1} + \mathbf{b}_i \otimes \hat{\mathbf{m}}_i^*. \tag{A2}$$

The averaged Young measure of the entire microstructure is a convex combination of Dirac masses with support on $\mathbf{A}_i$ and $\mathbf{B}_i$. Using the minors relations for homogeneous boundary conditions (2.18), we find that for some $\lambda_i \geq 0$ satisfying $\sum_{i=1}^{n} \lambda_i = 1$

$$\text{(i)} \quad \mathbf{F}_o = \sum_{i=1}^{n} \lambda_i (\mu_i \mathbf{B}_i + (1-\mu_i)\mathbf{A}_i) = \sum_{i=1}^{n} \lambda_i(\mathbf{1} + \mathbf{b}_i \otimes \mathbf{m}_i),$$

$$\text{(ii)} \quad \operatorname{cof}\mathbf{F}_o = \sum_{i=1}^{n} \lambda_i (\mu_i \operatorname{cof}\mathbf{B}_i + (1-\mu_i)\operatorname{cof}\mathbf{A}_i) \quad \text{and}$$

$$\text{(iii)} \quad \det\mathbf{F}_o = \sum_{i=1}^{n} \lambda_i (\mu_i \det\mathbf{B}_i + (1-\mu_i)\det\mathbf{A}_i).$$

Because $\mathbf{B}_i - \mathbf{A}_i = \mathbf{a}_i \otimes \hat{\mathbf{n}}_i$, from (2.19) and (A2),

$$\mu_i \operatorname{cof}\mathbf{B}_i + (1-\mu_i)\operatorname{cof}\mathbf{A}_i = \operatorname{cof}(\mu_i \mathbf{B}_i + (1-\mu_i)\mathbf{A}_i) = \operatorname{cof}(\mathbf{1} + \mathbf{b}_i \otimes \mathbf{m}_i) \quad \text{and}$$

$$\mu_i \det\mathbf{B}_i + (1-\mu_i)\det\mathbf{A}_i = \det(\mu_i \mathbf{B}_i + (1-\mu_i)\mathbf{A}_i) = \det(\mathbf{1} + \mathbf{b}_i \otimes \mathbf{m}_i).$$

Therefore,

$$\text{(i)} \quad \mathbf{F}_o = \sum_{i=1}^{n} \lambda_i(\mathbf{1} + \mathbf{b}_i \otimes \mathbf{m}_i),$$

$$\text{(ii)} \quad \operatorname{cof}\mathbf{F}_o = \sum_{i=1}^{n} \lambda_i \operatorname{cof}(\mathbf{1} + \mathbf{b}_i \otimes \mathbf{m}_i) \quad \text{and} \tag{A3}$$

---

* Notice that this assumption does not follow for the inner sets of fine twins from the jump condition in Figure A1a. However, we assume this as a part of the plate group idea.

(iii) $\det \mathbf{F}_o = \sum_{i=1}^{n} \lambda_i \det (\mathbf{1} + \mathbf{b}_i \otimes \mathbf{m}_i)$.

These conditions are necessary for coherence. It turns out that they are violated. One can verify that directly or use the following argument. We recall the identities,

(i) $\operatorname{cof} \mathbf{G} = (\det \mathbf{G})\, \mathbf{G}^{-1}$ if $\det \mathbf{G} \neq 0$,

(ii) $\det (\mathbf{1} + \mathbf{b} \otimes \mathbf{m}) = 1 + \mathbf{b}\cdot\mathbf{m}$ and

(iii) $(\mathbf{1} + \mathbf{b} \otimes \mathbf{m})^{-1} = \mathbf{1} - \dfrac{\mathbf{b} \otimes \mathbf{m}}{1 + \mathbf{b}\cdot\mathbf{m}}$ if $\mathbf{b}\cdot\mathbf{m} > -1$.

Substituting these in (A3)(ii), we obtain

$$(\det \mathbf{F}_o)\, \mathbf{F}_o^{-1} = \Big(1 + \sum_{i=1}^{n} (\lambda_i \mathbf{b}_i \cdot \mathbf{m}_i) \Big)\, \mathbf{1} - \sum_{i=1}^{n} (\lambda_i\, \mathbf{b}_i \otimes \mathbf{m}_i).$$

Substituting from (A3)(iii),

$$(\det \mathbf{F}_o)\, \mathbf{F}_o^{-1} = (1 + \det \mathbf{F}_o)\, \mathbf{1} - \mathbf{F}_o.$$

Post-multiplying by $\mathbf{F}_o$ and rearranging,

$$\mathbf{F}_o^2 - (1 + \det \mathbf{F}_o)\mathbf{F}_o + (\det \mathbf{F}_o)\, \mathbf{1} = 0.$$

From this we can conclude that the eigenvalues of $\mathbf{F}_o$ are $\{1,\ 1$ and $\det \mathbf{F}_o\}$. Hence, if $\mathbf{F}_o$ is symmetric, it is of the form $\mathbf{1} + \mathbf{a} \otimes \mathbf{a}$ for some vector $\mathbf{a}$.

In each of the cases studied by Saburi and Wayman, n = 4 and $\lambda_i = \frac{1}{4}$ and

$$\mathbf{F}_o = \sum_{i=1}^{n} \tfrac{1}{4} (\mathbf{1} + \mathbf{b}_i \otimes \mathbf{m}_i) \text{ is of the form } \begin{bmatrix} 1+\alpha & 0 & 0 \\ 0 & 1+\beta & \gamma \\ 0 & \gamma & 1+\beta \end{bmatrix}. \qquad \text{(A4)}$$

Therefore $\mathbf{F}_o$ is symmetric and it has to be of the form $\mathbf{1} + \mathbf{a} \otimes \mathbf{a}$. This is true if and only if

$$\alpha = 0 \text{ and } \beta^2 = \gamma^2 \quad \text{or} \quad \beta = \gamma = 0. \qquad \text{(A5)}$$

However α, β, and γ are non-zero, though small. Thus the minors relation are violated and a plate group can not form a coherent (according to the concept of coherence used here) microstructure that satisfies homogeneous boundary conditions.

It may be argued that in the above examples α, β, and γ are small and their non-zero values reflect round-off errors errors during calculation and the errors in the measurement of lattice parameters. To clarify this, let us examine the cubic to tetragonal case in more detail. In this case, there are three variants of martensite and the transformation strain is given by (5.1). Wechsler, Leiberman and Read[69] have derived explicit solutions to (A1) for this case. However, the fomulae of Ball and James[9] which are in the format being followed here are used for the calculations. It is easy to verify that in the cubic basis $\{\hat{\mathbf{i}}_1,\hat{\mathbf{i}}_2,\hat{\mathbf{i}}_3\}$ described above, the following vectors $\mathbf{b}_i$ and $\hat{\mathbf{m}}_i$, i = 1, .. , 4 solve (A1) and potentially form a plate group.

$$\mathbf{b}_{1,2} = \rho\,\frac{1-\eta_1^2}{1+\eta_2}\left\{\pm\frac{\delta-\tau}{2},\ \frac{\delta+\tau}{2},\ -\eta_2\right\} \qquad \text{and} \qquad \hat{\mathbf{m}}_{1,2} = \frac{1}{\rho}\left\{\pm\frac{\delta-\tau}{2},\ \frac{\delta+\tau}{2},\ 1\right\}$$

$$\mathbf{b}_{3,4} = \rho\,\frac{1-\eta_1^2}{1+\eta_2}\left\{\pm\frac{\delta-\tau}{2},\ -\eta_2,\ \frac{\delta+\tau}{2}\right\} \qquad \text{and} \qquad \hat{\mathbf{m}}_{3,4} = \frac{1}{\rho}\left\{\pm\frac{\delta-\tau}{2},\ 1,\ \frac{\delta+\tau}{2}\right\}$$

$$\text{where } \delta = \sqrt{\frac{\eta_1^2+\eta_2^2-2}{1-\eta_1^2}}, \qquad \tau = \sqrt{\frac{2\eta_1^2\eta_2^2-\eta_1^2-\eta_2^2}{1-\eta_1^2}},$$

and $\rho \neq 0$ is chosen to make $|\hat{\mathbf{m}}_i| = 1$.

Therefore,

$$\sum_{i=1}^{n}\lambda_i(\mathbf{1}+\mathbf{b}_i\otimes\mathbf{m}_i) = \frac{1-\eta_1^2}{4\,(1+\eta_2)}\begin{bmatrix} 1+(\delta-\tau)^2 & 0 & 0 \\ 0 & 1+\frac{1}{2}\left((\delta+\tau)^2-4\eta_2\right) & (1-\eta_2)(\delta+\tau) \\ 0 & (1-\eta_2)(\delta+\tau) & 1+\frac{1}{2}\left((\delta+\tau)^2-4\eta_2\right) \end{bmatrix}$$

which is of the form (A4). Therefore, in order to satisfy the minors relation, (A5) must hold. A straight forward calculation reveals that any solution requires that $\eta_1 = 1$ or $\eta_2 = 1$. This is precisely the condition that allows us to form an interface between the austenite and a single variant of martensite and one that we saw is very rarely true. Thus, it is not possible to form a coherent

microstructure that satisfies homogeneous boundary conditions using, in equal proportion, the four sets of fine twins from any plate group.

Tas et al. as well as Saburi and Wayman found that $\mathbf{F}_o$ is close to $\mathbf{1}$ and concluded that the microstructure is self-accommodating. However, $\mathbf{F}_o$ is not of the form $\mathbf{1} + \mathbf{a} \otimes \mathbf{a}$. This means that the minors relations are violated which in turn means that not all the internal jump conditions are satisfied. If a microstructure which we know is coherent has an "average deformation gradient" close to $\mathbf{1}$, we can argue as we did in the end of Section 5 that it can be made to satisfy identity boundary conditions with small energy; but that is not the case here. Also, it may be possible to make an incoherent microstructure coherent at a small expense of energy. We were not possible to verify whether that is the case here.

In summary, the minors relations are a simple first check to determine whether it is possible to form a coherent microstructure that satisfies homogeneous boundary conditions using a given set of tensors. However, it should be emphasized that the satisfaction of the minors relation is a necessary, but not a sufficient, condition and hence, the satisfaction of minors relation is not a proof for the existence of microstructure.

ACKNOWLEDGEMENTS

I thank Richard D. James for his constant encouragement, numerous suggestions and for comments on an early draft. I am glad to acknowledge the support of the National Science Foundation and the Air Force Office of Scientific Research through NSF/DMS - 8718881 and the Academic Computing Services, University of Minnesota.

REFERENCES

1. Adachi, K. and Wayman, C.M., "Transformation behaviour of nearly stoichiometric Ni-Mn alloys" and "Electron microscopy study of θ-phase in Ni-Mn alloys", *Met.Trans. A* 16 A (1985), 1567-1579 and 1581-1597.

2. Andersen, N. H., Lebech, B. and Poulsen, H. F., "The structural phase diagram and oxygen equilibrium partial pressure of $YBa_2Cu_3O_{6+x}$ studied by powder diffraction and gas volumetry", *Physica C* 172 (1990), 31-42.

3. Arlt, G., "Twinning in ferroelectric and ferroelastic ceramics: stress relief", *J. Mat. Sci.* 22 (1990), 2655-2666.

4. Avellaneda, M., Cherkaev, A.V., Lurie, K.A. and Milton, G.W., "On the effective conductivity of polycrystals and a three dimensoinal phase-interchange inequality", *J. Appl. Phys.* 63 (1988), 4989-5003.

5. Ball, J.M., "Convexity conditions and existence theorems in nonlinear elasticity", *Arch. Rat. Mech. Anal.* 63 (1977), 337-403.

6. Ball, J.M., "Remarks on the paper 'Basic calculus of variations'", *Pacific J. Math* 116 (1985),7-10.

7. Ball, J.M., "A version of the fundamental theorem for Young measures", *PDEs and Continuum Models of Phase Transitions*(ed. Rascle, M., Serre, D. and Slemrod, M.), *Lecture Notes in Physics* 344 (1988), Springer -Verlag, 207-215.

8. Ball, J.M., Currie, J.C. and Olver, P.J., "Null Lagrangians, weak continuity and variational orders of arbitrary order", *J. Func. Anal.* 41 (1981), 135-174.

9. Ball, J.M. and James, R.D., "Fine phase mixtures as minimizers of energy", *Arch. Rat. Mech. Anal.* 100 (1989), 15-52.

10. Ball, J.M. and James, R.D., "Proposed experimental tests of a theory of fine microstructure and the two well problem", *Phil. Trans. Royal Soc. London A,* To appear (1991).

11. Ball, J.M. and Murat, F., "$W^{1,p}$ - quasiconvexity and variational problems for multiple integrals", *J. Func. Anal.* 58 (1984), 225-253.

12. Bhattacharya, K., "Wedge-like microstructure in martensite", *Acta Metall.* , To appear (1991).

13. Billington, E. W. and Tate, A., "The Physics of Deformation and Flow", Mc-Graw Hill 1960).

14. Birnbaum, H.K. and Read, T.A., "Stress induced twin boundary motion in AuCd β' and β" alloys", *Trans. Met. Soc. AIME* 218 (1960), 662-669.

15. Bowles, J.S. and MacKenzie, J.K., "The crystallography of martensitic transformations I and II", *Acta Metall.* 2 (1954), 129-137 and 138-147.

16. Bywater, K.A. and Christian, J.W., "Martensitic transformations in titanium-tantalum alloys", *Phil. Mag.* 25 (1972), 1249-1272.

17. Chakravorty, S. and Wayman, C.M., "The thermoelastic martensitic transformation in β' Ni-Al alloys: I. Crystallography and morphology and II.Electron microscopy", *Metall. Trans. A* 7A (1976), 555-568 and 569-582.

18. Chang, L.C. and Read, T. A., "Plastic deformation and diffusionless phase changes in metals - the gold-cadbium beta phase", *J. Metals Trans. AIME* 191 (1951), 47-52.

19. Chipot, M. and Kinderlehrer, D., "Equilibrium configurations of crystals", *Arch. Rat. Mech. Anal.* 103 (1988), 237-277.

20. Dacarogna, B., "Direct methods in the calculus of variations", Springer-Verlag(1988).

21. Enami, K. and Nenno, S., "Memory effect in Ni-36.8 at. pct. Al martensite",. *Metall. Trans.* 2 (1971), 1487-1490.

22. Ericksen, J.L., Nilpotent energies in liquid crystal theory, *Arch. Rat. Mech. Anal.* 10 (1962), 189-196.

23. Ericksen, J.L., "Nonlinear elasticity of diatomic crystals", *Int. J. Solids Struc.* 6 (1970), 951-957.

24. Ericksen, J.L., "Special topics in elastostatics", *Adv. Appl. Mech.* 7 (1977), Academic Press, 189-243.

25. Ericksen, J.L., "On the symmetry and stability of thermoelastic solids", *J. Appl. Mech.* 45 (1978), 740-744.

26. Ericksen, J.L., "On the symmetry of deformable crystals", *Arch. Rat. Mech. Anal.* 72 (1979), 1-13.

27. Ericksen, J.L., "The Cauchy and Born hypotheses for crystals", *Phase transformations and material instabilities in solids*(ed. Gurtin, M.), Academic Press (1984), 61-78.

28. Ericksen, J.L., "Constitutive theory for some constrained elastic crystals", *Int. J. Solids Struc.* 22 (1986), 951-964.

29. Ericksen, J.L., "Weak martensitic transformations in Bravais lattices", *Arch. Rat. Mech. Anal.* 107 (1989), 23-36.

30. Evans, L.C., "Weak Convergence Methods for Nonlinear Partial Differential Equations", *Am. Math. Soc.* CBMS 74 (1990).

31. Firoozye, N.B., Bhattacharya, K., James, R.D., Kohn, R.V., "Restrictions on microstructure", In preparation (1991).

32. Foos, M., Frantz, C. and Gantios, M., "Shape memory effect and anelasticity associated with the martensitic transformation in the stoichiometric Fe_3Pt alloy", *Shape Memory Effects in Alloys* (ed. Perkins, J.), Plenum Press (1975).

33. Forsbergh, P.W., "Domain structures and phase transitions in Barium Titanate", *Phys. Rev.* 76 (1949), 1187-1201.

34. Fosdick, R.L. and Hertog, B., "Material symmetry and crystals", *Arch. Rat. Mech. Anal.* 110 (1990), 43-72.

35. Guttman, L., "Crystal structures and transformations in Indium-Thallium solid solutions", *J. Metals Trans. AIME* 188 (1950), 1472-1477.

36. Hanson, C.G., Rivlin, V.G. and Hatt,B.A., "The β-phase transformation of some zirconium-thorium alloys", *J. Nuclear Mat.* 12 (1964), 83-93.

37. James, R.D., "Displacive phase transformations in solids", *J. Mech. Phys. Solids* 34 (1986), 359-394.

38. James, R.D., "The stability and metastability of quartz", *Metastability and incompletely posed problems* IMA Vol 3, Springer-Verlag (1987), 147-176.

39. James, R.D. and Kinderlehrer, D., "Theory of diffusionless phase transitions", *Partial Differential Equations and Continuum Models of Phase Transitions*(ed. Rascle, M., Serre, D. and Slemrod, M.), *Lecture Notes in Physics* 344, Springer-Verlag (1989), 51 - 84.

40. Kinderlehrer, D. and Pedregal, P., "Characterizations of Young measures generated by gradients", *Arch. Rat. Mech. Anal.*, To appear (1991).

41. Krasevec, V., "The complex microstructure in quenched Ni-Mn alloy", *Phys. Stat. Sol. A* 30 (1975), 241-250.

42. Kudoh, Y., Tokonami, M., Miyazaki, S. and Otsuka, K., "Crystal structure of the martensite in Ti 49.2 at % Ni alloy analysed by the single crystal X-ray diffraction method", *Acta Metall.* 33 (1985), 2049-2056.

43. Maki, T. and Tamura, I., *Proc. Int. Conf. Mart. Trans.* (1986), 963-970.

44. Masson, D.B. and Barrett, C.S., "Effect of deformation and low temperatures on the structure of AgCd and AuZn", *Trans. Met. Soc. AIME* 212 (1958), 260-265.

45. Miyazaki, S. and Otsuka, K., "Development of Shape Memory Alloys", *ISIJ Int.* 29 (1989), 353-377.

46. Miyazaki, S., Otsuka, K. and Wayman, C.M., "The shape memory mechanism associated with the martensitic transformation in TiNi alloys - I. Self-accommodation and II. Variant Coalescence and shape recovery", *Acta Metall.* 37 (1989), 1873-1884 and 1885-1890.

47. Morton, A.J. and Wayman, C.M., "Theoretical and experimental aspects of the "(225)" austenite-martensite transformation in iron alloys", *Acta Metall.* 14 (1967), 1567-1581.

48. Murakami, Y. and Kanchi, S., "Microscopic observation of thermoelastic α_2 Ni-Zn-Cu martenstite", *Trans. Jap. Inst. Metals* 18 (1977), 423-426.

49. Murakami, Y., Kanchi, S. and Shimizu, S., "Martensitic transformation and elastic properties of the ternary Ni-Zn β_2 base phase alloy", *Trans. Jap. Inst. Metals* 17 Suppl. (1976), 147-157.

50. Murat, F., "Compacite par compensation", *Ann. Sci. Norm. Sup. Pisa* 5 (1978), 489-507.

51. Murat, F., "Compacite par compensation II", *Recent Methods in Nonlinear Analysis*, (ed. De Giorgi, E., Magenes, E. and Mosco Pitagora, U.) (1979), 245-256.

52. Murat, F. and Tartar, L., "Calcul des variations et homogeneisation, Les Methodes de l'homogeneisation: Theorie et Applications en Physique", *Dir. des Etudes et Recherches de l'EDF*, Eyrolles, Paris (1985), 319-370.

53. Nittono, O. and Koyoma, Y., "Crystal structure and phase transformations in Indium rich solid solution", *Sci. Rep. Research Inst. Tohoku U.* A 29 Suppl. 1 (1981), 53-60.

54. Okamoto, H., Oka, M. and Tamura, I., "Coupling of thin-plate martensites in an Fe-Ni-C alloy", *Trans. Jap. Inst. Metals* 19 (1978), 674-684.

55. Okamoto, K., Ichinose, S., Morii, K., Otsuka, K. and Shimizu, K, "Crystallography of β_1 - γ'_1 stress induced martensitic transformation in a Cu-Al-Ni alloy", *Acta Metall.* 34 (1986), 2065-2073.

56. Pitteri, M., "Reconciliation of the local and global symmetries of crystals", *J. Elasticity* 14 (1984), 175-190.

57. Pitteri, M., "On ν+1-lattices", *J. Elasticity* 15 (1985), 3-25.

58. Saburi,T. and Wayman, C.M., "Crystallographic similarities in shape memory martensites", *Acta Metall.* 27 (1977), 976-995.

59. Serre, D., "Formes quadratiques et calcul des variations", *J. Math. Pures. Appl.* 62 (1983), 117-196.

60. Sohmura, T., Oshima, R. and Fujita, F.E., "Thermoelastic FCC-FCT transformation in martensitic transformation in Fe-Pd alloys", *Scripta Met.* 14 (1980), 855-856.

61. Subbarao, E.C., "Zirconia - an overview", *Science and Technology of Zirconia* (ed. Heuer, A.H. and Hobbs, L.W.), *Adv. in Ceramics* 3 (1980), 1-24.

62. Tadaki, T. and Shimizu, K., "High tetragonality of the thermoelastic martensitic transformation and small volume change during the transformation", *Scripta Metall.* 9 (1975), 771-776.

63. Tan, S. and Xu, H., "Observations on a CuAlNi single crystal", *Cont. Mech. Thermodynamics* 2 (1990), 241-244.

64. Tartar, L., "Compensated compactness and applications to partial differential equations", *Nonlinear Analysis and Mechanics* (ed. Knops, R.J.), *Research Notes* 39 (1978), Pittman, London, 136-212.

65. Tas, H., Delaey, L. and Deruytere, A., "The self-accommodating character of the β'_1 copper aluminum martensite", *Metall. Trans.* 4 (1973), 2833-2840.

66. Van Tendeloo, G. and Amelinckx, S., "Group theoretical considerations concerning domain formation in ordered alloys", *Acta Cryst.* A30 (1974), 431.

67. Van Tendeloo, G., Private Communication (1991).

68. Watanabe, M. and Wayman, C.M., "Crystallography of the martensite transformation in Fe-Al-C alloys", *Metall. Trans.* 2 (1971), 2229-2236.

69. Wechsler, M.S., Lieberman, D.S. and Read, T.A., "On the theory of the formation of martensite", *J. Metals Trans. AIME* 197 (1953), 1503-1515.

70. Wheeden, R.L. and Zygmund, A., "Measure and integral: An introduction to real analysis", Marcel Dekker Inc (1977).

71. Zanzotto, G. "On the material symmetry group of elastic crystals and the Born rule", To appear.

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